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ch level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom

H,F,CH3,NH2,SH

14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 65:CLASS 67:CLASS 68:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:CLASS 77:CLASS 77:CLASS 79:CLASS 81:CLASS 82:CLASS 84:CLASS 85:CLASS 86:CLASS 88:CLASS 89:CLASS 91:CLASS 92:CLASS 93:CLASS 95:CLASS 97:CLASS 98:CLASS

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FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004

=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

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STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

=> L1

STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

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=> s 11

SAMPLE SEARCH INITIATED 00:32:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS

25 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS:

4998 TO 7082

PROJECTED ANSWERS:

200 TO 800

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:32:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

100.0% PROCESSED 6058 ITERATIONS

447 ANSWERS

SEARCH TIME: 00.00.01

L3 447 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 168.44 168.65

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004
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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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1 L4 AND PRIESTLEY, E?/AU L5

=> d 15, ibib abs fhitstr, 1

ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full References

ACCESSION NUMBER:

2003:261620 HCAPLUS

DOCUMENT NUMBER:

138:287673

TITLE:

Preparation of phenylbenzimidazole compounds useful

for treating hepatitis C virus

INVENTOR (S):

Priestley, Eldon Scott; Decicco, Carl. P.; Hudyma,

Thomas W.; Zheng, Xiaofan

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA PCT Int. Appl., 74 pp.

SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.				KI	ND 1	DATE			AI	PPLIC	CATIO	ON NO	). I	DATE				
	WO	2003	02658	<u> 37</u>	A2	2 :	2003	0403		WC	200	)2-US	3098	39	20020	926			
	WO	2003	02658	37	A.	3	2003	1106								-			
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	ΒA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	ΕĒ,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JΡ,	KE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	
			UA,	UG,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,	ΤJ,	TM
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	ВG,	
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					TD,														
	US	2003	1348	53	A.	1	2003	0717		U:	S 200	02-2	5904	<u>L</u>	2002	0926			
	US	2004	0679	76	A:	1 .	2004	0408		U	5 200	03-64	1887	3_	2003	0827			
PRIOR	ITY	APP	LN.	INFO	. :				]	US 2	001-3	3248	74P	P	2001	0926			
									1	US 2	002-2	25904	<u> 1 1 </u>	B1	2002	0926			
OTHER	SO	URCE	(S):			MAR	PAT	138:2	2876	73									

AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14  $\mu$ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 503857-56-5 HCAPLUS

CN Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN <u>503857-55-4</u> CMF C40 H41 N7 O5 S

CM 2

CRN <u>76-05-1</u> CMF C2 H F3 O2

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(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

STRUCTURE UPLOADED L1

L225 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

13 S L3 L4

1 S L4 AND PRIESTLEY, E?/AU L5

=> s 14 not 15

12 L4 NOT L5

=> s 16 and decicco, c?/au

125 DECICCO, C?/AU

0 L6 AND DECICCO, C?/AU L7

=> s 16 and hudyma, t?/au

45 HUDYMA, T?/AU

0 L6 AND HUDYMA, T?/AU 1.8

=> s 16 and zheng, x?/au

3518 ZHENG, X?/AU

0 L6 AND ZHENG, X?/AU L9

=> d 16, ibib abs fhitstr, 1-12

ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN L6

Full References Text ACCESSION NUMBER:

2003:981461 HCAPLUS

DOCUMENT NUMBER:

140:246106

Non-nucleoside inhibitors of the hepatitis C virus TITLE:

NS5B polymerase: discovery and preliminary SAR of

benzimidazole derivatives

Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; AUTHOR (S):

Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet,

Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin,

Charles; Austel, Volkhard; Kukolj, George

Department of Chemistry, Research and Development, CORPORATE SOURCE:

Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S

2G5, Can.

Bioorganic & Medicinal Chemistry Letters (2004), SOURCE:

14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

Benzimidazole 5-carboxamide derivs. from a combinatorial screening library AΒ were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

IT 390815-16-4P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

390815-16-4 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN L6

ACCESSION NUMBER:

2003:319709 HCAPLUS

DOCUMENT NUMBER:

138:338144

TITLE:

Preparation of 2-phenyl benzimidazoles and

imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the

treatment of cancer

INVENTOR(S):

Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J.

Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.

PATENT ASSIGNEE(S):

Ortho-McNeil Pharmaceutical, Inc., USA

PCT Int. Appl., 144 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DAT	TE	APPLICATION N	O. DATE	
***************************************		030424	WO 2002-US333	371 20021	018
WO 2003032984	A1 200	030424	WO 2002-03333	20023	.010
WO 2003032984		031120			
W: AE, AG	AL, AM, AT	T, AU, AZ,	BA, BB, BG, BR,	, BY, BZ,	CA, CH, CN,
			DZ, EC, EE, ES,		
GM, HR	HU, ID, II	L, IN, IS,	JP, KE, KG, KP,	, KR, KZ,	LC, LK, LR,
LS. LT	LU, LV, MA	A, MD, MG,	MK, MN, MW, MX,	, MZ, NO,	NZ, OM, PH,

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PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
    US 2003176438
                            20030918
                                           US 2002-273487
                                                             20021018
                       A1
                            20030818
                                           NO 2003-2759
                                                             20030617
    NO 2003002759
                       Α
                                        US 2001-330304P
                                                             20011019
PRIORITY APPLN. INFO.:
                                        WO 2002-US33371
                                                          W
                                                             20021018
                         MARPAT 138:338144
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OTHER SOURCE(S):

Ι

GT

2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; AB e.g. 2-[4-(4-chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cds1 and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(0)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1 or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Ar1 is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide. Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example prepns. are included.

IT 516480-80-1P, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5-

carboxylic acid

RN

CN

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

516480-80-1 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2004 ACS on STN L6 ANSWER 3 OF 12

ACCESSION NUMBER:

2003:203407 HCAPLUS

DOCUMENT NUMBER:

138:238181

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

Japan Tobacco Inc., Japan

SOURCE:

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT 1	NO.		KIND DATE					A	PPLI	CATIO	ON NO	٥.	DATE			
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1	US 2003	0503	20	A	1 :	2003	0313		U	S 20	01-9	3937	4	2001	0824		
1	WO 2001	0478	83	A	1	2001	0705		W	0 20	00-J	P918	1	2000	1222		
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		CR,	CU,	ÇΖ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
		HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
		MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
		SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	ŪG,	US,	UZ,	VN,	YU,	ZA,	
		AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	ΤJ,	TM							
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	JP 2001	2475	50	A:	2	2001	0911		J	P 20	00-3	9190	4	2000	1225		
PRIOR	ITY APP	INFO	. :					JP 1	999-	3690	80	Α	1999	1227			
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						1	JP 2	000-	3919	04	A	2000	1225				
								1	JP 2	001-	1937	86	Α	2001	0626		
OTHER	SOURCE	(S):			MAR	PAT	138:	2381	81								

GΙ

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy =(un) substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data

given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1cyclohexylbenzimidazole-5-carboxylate, was given.

IT 347165-35-9P

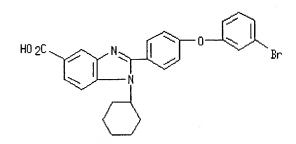
CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

347165-35-9 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1cyclohexyl- (9CI) (CA INDEX NAME)



ANSWER 4 OF 12 **HCAPLUS** COPYRIGHT 2004 ACS on STN L6

Citing Reference Full

ACCESSION NUMBER:

2003:5773 HCAPLUS

DOCUMENT NUMBER:

138:66657

TITLE: INVENTOR (S): Fused cyclic compounds and medicinal use thereof Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

SOURCE:

Japan Tobacco Inc., Japan PCT Int. Appl., 603 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.		KI	ND :	DATE			Al	PPLI	CATIO	ои ис	٥.	DATE			
WO 20030002	54	A:	 1	2003	0103		W	20	02-J	P640!	5	20020	0626	-	
W: AE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
GM,	HR,	HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	KΖ,	LC,	LK,	LR,	LS,	LT,
LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	PL,	PT,
RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,
US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM
RW: GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,
CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
JP 20032128	46	A:	2	2003	0730		<u>J</u> 1	P 20	02-1	8524	1_	2002	0625		
BR 20020056															
EP 1400241	EP 1400241 A1 200403						E	P 20	02-7	4372	<u> 8</u>	2002	0626		
R: AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	ΝL,	SE,	MC,	PT,
IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR						
<u>US 2004082635</u> A1 20040429							<u>U</u> :	S 20	03-34	4499	7	2003	218		
NO 2003000832 A 20030422							N	20	03-8	32		2003	221		

5/12/04

PRIORITY APPLN. INFO.:

JP 2001-193786 A 20010626

A 20011116

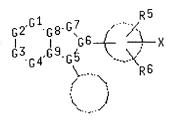
JP 2001-351537 WO 2002-JP6405

W 20020626

OTHER SOURCE(S):

MARPAT 138:66657

GΙ



I

Fused cyclic compds. represented by the following general formula [I] or AΒ pharmaceutically acceptable salts thereof and remedies for hepatitis C contq. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

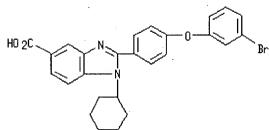
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

347165-35-9 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-CNcyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS 27 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References Text ACCESSION NUMBER:

2002:51438 HCAPLUS

DOCUMENT NUMBER: 136:118447

Preparation of benzimidazolecarboxylates and related TITLE:

compounds as viral polymerase inhibitors

Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James; INVENTOR(S):

Kukolj, George; Austel, Volkhard

Boehringer Ingelheim (Canada) Ltd., Can. PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2002004425 20020117 WO 2001-CA989 20010704 A2 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 2002065418 Α1 20020530 US 2001-898297 US 6448281 20020910 B2 EP 1301487 A2 20030416 EP 2001-951274 20010704 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR JP 2004502761 T2 20040129 JP 2002-509292 20010704 US 6479508 В1 20021112 US 2001-995099 20011127 WO 2002070739 A2 20020912 WO 2002-CA323 20020306 WO 2002070739 A3 20030530 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ. TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG EP 1370682 A2 20031217 EP 2002-712681 20020306 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2003232816 A1 20031218 US 2002-238282 20020910 PRIORITY APPLN. INFO.: US 2000-216084P P 20000706 US 2001-274374P P 20010308 US 2001-281343P P 20010405 US 2001-898297 A3 20010703 WO 2001-CA989 W 20010704 US 2001-995099 A3 20011127 WO 2002-CA323 W 20020306 OTHER SOURCE(S): MARPAT 136:118447

GI

AB Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH2, NMeR3, NHR3, OR3, 5-6
 membered (substituted) heterocyclyl; A = N, COR7, CR5; R5 = H, halo,
 alkyl; R7 = H, alkyl; X and A are not both N; R6 = H, halo, alkyl, OR7; R7
 = H, alkyl; R1 = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl,
 alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF3; R2 = (substituted) alkyl,

cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5  $\mu$ M.

IT 347166-09-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN347166-09-0 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-CN(phenylmethoxy)phenyl] - (9CI) (CA INDEX NAME)

ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

eille" Full References Text

2001:489367 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

135:76874

Preparation of heterocyclic compounds as remedies for TITLE:

hepatitis C

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, INVENTOR(S):

Atsuhito

PATENT ASSIGNEE(S):

SOURCE:

Japan Tobacco Inc., Japan PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DAT	E	APPLICATI	ON NO.	DATE					
WO 2001047883	A1 200	10705	WO 2000-J	P9181	20001222					
W: AE, AG,	AL, AM, AT	, AU, AZ,	BA, BB, BG,	BR, BY	BZ, CA,	CH, CN,				
CR, CU,	CZ, DE, DK	, DM, DZ,	EE, ES, FI,	GB, GD	GE, GH,	GM, HR,				
HU, ID,	IL, IN, IS	, KE, KG,	KR, KZ, LC,	LK, LR	LS, LT,	LU, LV,				
MA, MD,	MG, MK, MN	, MW, MX,	MZ, NO, NZ,	PL, PT	, RO, RU,	SD, SE,				
SG, SI,	SK, SL, TJ	, TM, TR,	TT, TZ, UA,	UG, US	UZ, VN,	YU, ZA,				
ZW, AM,	AZ, BY, KG	, KZ, MD,	RU, TJ, TM							
RW: GH, GM,	KE, LS, MW	, MZ, SD,	SL, SZ, TZ,	UG, ZW	AT, BE,	CH, CY,				
			IE, IT, LU,							
BJ, CF,	CG, CI, CM	, GA, GN,	GW, ML, MR,	NE, SN	TD, TG					
EP 1162196	A1 200	11212	EP 2000-9	EP 2000-987728 20001222						

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

	- •		
BR 2000008525	Α	20020102	BR 2000-8525 20001222
TR 200103147	T1	20020621	TR 2001-20010314720001222
NZ 514403	A	20021025	NZ 2000-514403 20001222
AU 763356	B2	20030717	AU 2001-24017 20001222
RU 2223761	C2	20040220	RU 2001-126283 20001222
NO 2001004134	Α	20011022	NO 2001-4134 20010824
US 2003050320	A1	20030313	<u>US 2001-939374</u> 20010824
ZA 2001007870	Α	20020925	ZA 2001-7870 20010928
PRIORITY APPLN. INFO.:			JP 1999-369008 A 19991227
			WO 2000-JP9181 W 20001222
			JP 2000-391904 A 20001225
			JP 2001-193786 A 20010626

OTHER SOURCE(S):

MARPAT 135:76874

GΙ

HO 
$$2^{\mathbb{C}}$$

N

O-CH  $2$ 

Me

II

The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011  $\mu$ M against hepatitis C virus polymerase. A formulation is given.

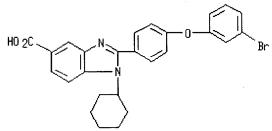
IT 347165-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS 27 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN L6 ANSWER 7 OF 12 HCAPLUS

Full

ACCESSION NUMBER:

2001:412102 HCAPLUS

DOCUMENT NUMBER:

135:177890

TITLE:

Synthesis and antimicrobial activity of some new 2-phenyl-N-substituted carboxamido-1H-benzimidazole

derivatives

AUTHOR(S):

SOURCE:

Goker, Hakan; Tuncbilek, Meral; Suzen, Sibel; Kus,

Canan; Altanlar, Nurten

CORPORATE SOURCE:

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk. Archiv der Pharmazie (Weinheim, Germany) (2001),

334(5), 148-152

CODEN: ARPMAS; ISSN: 0365-6233

PUBLISHER:

Wiley-VCH Verlag GmbH

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 135:177890

GI

Some 1H-benzimidazole-carboxamide derivs. were prepd. and their AB antimicrobial activities against Staphylococcus aureus, Escherichia coli, and Candida albicans evaluated. Compds. I, II, and III exhibited the best activity against C. albicans.

IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antimicrobial activity of new 2-phenyl-N-substituted carboxamido-1H-benzimidazole derivs.)

174422-18-5 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) CN (CA INDEX NAME)

0 – CH 2– Ph

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN L6

8

Citie Full Text References

ACCESSION NUMBER:

1999:614608 HCAPLUS

DOCUMENT NUMBER:

131:286454

TITLE:

Synthesis and antimicrobial activity of some new

benzimidazole carboxylates and carboxamides

AUTHOR (S):

Ayhan-Kilcigil, Gulgun; Tuncbilek, Meral; Altanlar,

Nurten; Goker, Hakan

CORPORATE SOURCE:

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.

Farmaco (1999), 54(8), 562-565

SOURCE: CODEN: FRMCE8; ISSN: 0014-827X

Elsevier Science S.A. PUBLISHER:

DOCUMENT TYPE:

Journal

LANGUAGE:

English

GT

Benzimidazole carboxylates and carboxamides, e.g., I [R1 = MeO, AB (2-pyridinylmethyl)amino, 4-methylpiperidino, R2 = 2-ClC6H4, 4-ClC6H4, 2,4-Cl2C6H3, 2-MeOC6H4, 4-MeOC6H4, 2-thienyl], were synthesized and evaluated for their antimicrobial activities against Staphylococcus aureus, Escherichia coli, and Candida albicans. Among the investigated compds., I (R1 = MeO, R2 = 2-MeOC6H4) exhibited best activity against C. albicans.

IT 246517-85-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and antimicrobial activity of benzimidazole carboxylates and carboxamides)

246517-85-1 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]-1-CN

(phenylmethyl) -, methyl ester (9CI) (CA INDEX NAME)

MeO - C N N CH 2-Ph

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER:

1999:184240 HCAPLUS

DOCUMENT NUMBER:

130:209707

TITLE:

Preparation of 2-substituted phenyl-benzimidazole

antibacterial agents

INVENTOR(S):

Ohemeng, Kwasi Adomako; Nguyen, Van Nhatton

Ortho-McNeil Pharmaceutical, Inc., USA

SOURCE:

PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT	NO.		KIND DATE				A.	BBPT.	CATI	J. 1	. DATE					
					<del>-</del> -			-								
WO 991	1627		A	1	1999	0311		W	0 19	98-U	S185	86	1998	0904		
W:	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
•	DK,	EE,	ES,	FI,	GB,	GE,	GH,	HU,	IL,	IS,	JP,	KΕ,	KG,	KP,	KR,	KΖ,
	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,
	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	UA,	UG,	UΖ,
	VN,	YU,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM				
RW	RW: GH, GM,					SD,	SZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,	DK,	ES,
	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВĴ,	CF,	CG,	CI,
						MR,	NE,	SN,	TD,	TG					•	
(US 594	2532 <sup>3</sup>	)	A	,	1999	0824		U	S 19	97-9	2455	8	1997	0905		
AU 989	3054	,	Α	1	1999	0322		A	U 19	98-9	3054		1998	0904		
PRIORITY AP	INFO	. :					US 1	997-	9245	58		1997	0905			
			•					WO 1	998-	US18.	586		1998	0904		

OTHER SOURCE(S):

MARPAT 130:209707

GT

$$R^{5}$$
 $R^{7}$ 
 $R^{1}$ 
 $R^{2}$ 
 $R^{3}$ 
 $R^{4}$ 
 $R^{4}$ 

AB Benzimidazoles I [R1 = H, OH, alkoxy; R2, R3, R4 = H, OH, alkyl, CF3, halo, etc.; R5 = H, amino, amidino; R6 = nitro, C(NHR9):NR10; R7 = H, amino, nitro; R8 = H, Me], antibacterial compds., were prepd. These compds. are effective in inhibiting the action of a bacterial histidine protein kinase and are useful as anti-infective agents against a variety

of bacterial organisms, including organisms which are resistant to other known antibiotics. E.g., 3,4-diaminobenzimidate, prepd. from 3,4-diaminobenzonitrile, was treated with NH3/EtOH, then with 4-Me3CC6H4CHO to give 2-[4-(1,1-dimethylethyl)phenyl]-2H-benzimidazole-5carboximidamide.

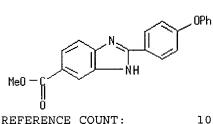
## IT 220955-73-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylbenzimidazoles as antibacterial agents)

220955-73-7 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-(4-phenoxyphenyl)-, methyl ester CN(9CI) (CA INDEX NAME)



103(a) Bioisosferl

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER:

1998:634393 HCAPLUS

DOCUMENT NUMBER: 129:316174

Synthesis of some new benzimidazolecarboxamides and TITLE:

evaluation of their antimicrobial activity

Goker, Hakan; Tuncbilek, Meral; Ayhan, Gulgun; AUTHOR (S):

Altanlar, Nurten

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of

Pharmacy, Ankara University, Ankara, 06100, Turk.

Farmaco (1998), 53(6), 415-420 SOURCE:

CODEN: FRMCE8; ISSN: 0014-827X

Elsevier Science S.A. PUBLISHER:

Journal DOCUMENT TYPE: English LANGUAGE:

A series of 1,2-disubstituted benzimidazole-5(6)-carboxamides was prepd. and evaluated in vitro for antimicrobial activity against Staphylococcus aureus, Escherichia coli, and Candida albicans. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids with aldehydes and via several steps over the 2(1H)-benzimidazolones, resp. All acids were converted to their acyl chlorides with SOC12, then amidified with several N, N'-dialkylaminoethyl derivs.

## IT 174422-18-5

RL: RCT (Reactant); RACT (Reactant or reagent) (prepn. and bactericidal and fungicidal activity of benzimidazolecarboxamides)

RN174422-18-5 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) CN (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1996:144268 HCAPLUS

DOCUMENT NUMBER:

124:197998

TITLE:

Synthesis of 1,2-disubstituted benzimidazole-5(6)carboxamides and evaluation of their antimicrobial

activity

AUTHOR (S):

Goeker, Hakan; Tebrizli, Emin; Abbasoglu, Ufuk

CORPORATE SOURCE:

Faculty of Pharmacy, Univ. of Ankara, Tandogan, 06100,

SOURCE:

Farmaco (1996), 51(1), 53-8

CODEN: FRMCE8

PUBLISHER:

Societa Chimica Italiana

DOCUMENT TYPE:

Journal

LANGUAGE:

English

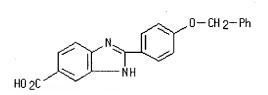
Fourteen N'-(N,N-dialkylaminoethyl)-benzimidazole 5(6)- or 5-carboxamides having several substituents on the azole and benzene nuclei were prepd. and evaluated in vitro for antimicrobial activity. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids and several aldehydes with cupric ion. carboxamides were prepd. from the corresponding acids and N, N-dialkylethylenediamine. Antibacterial and antifungal activities were detd. as MIC values. Compds. which were prepd. by replacement with bulky alkyl groups on the tert-N benzimidazole atom gave the best results.

IT 174422-18-5P

RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity)

RN 174422-18-5 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) CN(CA INDEX NAME)





L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on

Citing Full ACCESSION NUMBER:

1996:38013 HCAPLUS

DOCUMENT NUMBER:

124:202112

TITLE:

Synthesis of some new benzimidazole-5(6)-carboxylic

acids

AUTHOR (S):

Goeker, Hakan; Oelgen, Suereyya; Ertan, Rahmiye;

Akquen, Huelya; Oezbey, Sueheyla; Kendi, Engin; Topcu,

Guel

CORPORATE SOURCE:

SOURCE:

Fac. Pharmacy, Ankara Univ., Ankara, 06100, Turk. Journal of Heterocyclic Chemistry (1995), 32(6),

1767-73

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER:

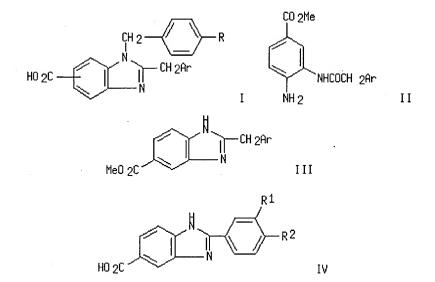
DOCUMENT TYPE:

LANGUAGE:

GI

HeteroCorporation

Journal English



AB The title compds., 1,2-dialkyl-benzimidazole-5(6)-carboxylic acids I (Ar = Ph, 4-MeC6H4, 4-ClC6H4, 2-BrC6H4, OPh, 4-ClC6H4O, etc., R = H, F, CO2H position = 5, 6) were prepd. in four steps; (1) prepn. of mono amide derivs. II by the reaction of Me 3,4-diaminobenzoate and substituted Ph or phenoxyacetic acid chlorides ArCH2COC1, (2) prepn. of the Me benzimidazolecarboxylates III, with zinc chloride and dry hydrogen chloride gas, (3) alk. hydrolysis of the esters, and (4) substitution of the imidazole ring with benzyl or p-fluorobenzyl bromide, in alkali medium. 2-Aryl-benzimidazole-5(6)-carboxylic acids IV (R1 = H, OCH2Ph, OH, R2 = OCH2Ph, OH) were prepd. via the oxidative condensation of 3,4-diaminobenzoic acid and arom. aldehydes with cupric ion.

## IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazolecarboxylic acids)

RN174422-18-5 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) CN(CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

SINCE FILE TOTAL
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-9.01

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

#### => d his

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FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

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L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU

L8 0 S L6 AND HUDYMA, T?/AU

L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

=> s 13

L10 0 L3

=> file req

COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

CA SUBSCRIBER PRICE

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <u>HELP PROP</u> at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

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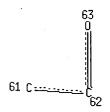
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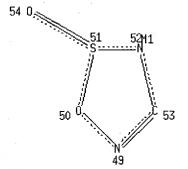
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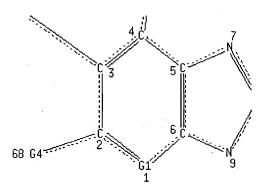
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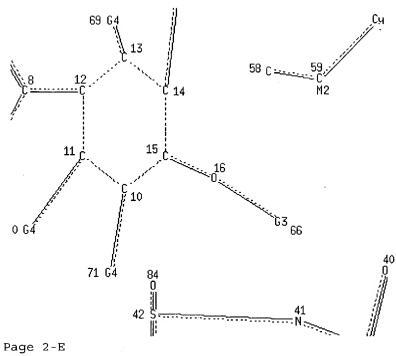


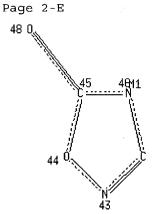
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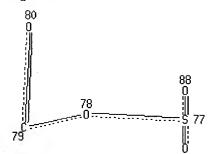
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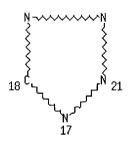


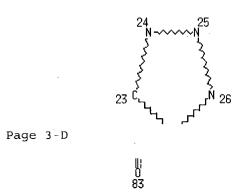


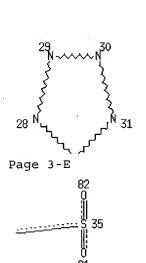
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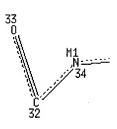
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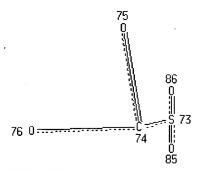




Page 3-F



87



Page 4-B



Page 4-D



Page 4-E

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VAR G2=18/24/29/35/36/42/47/53/73/77

VAR G3=91/57/58/61/64

VAR G4=92/93/94/95

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NUMBER OF NODES IS 95
STEREO ATTRIBUTES: NONE
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SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE
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                                                                    37 ANSWERS
100.0% PROCESSED
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                          BATCH **COMPLETE**
PROJECTED ITERATIONS: 4998 TO 7082
PROJECTED ANSWERS:
                                 376 TO 1104
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L12
=> s 111 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
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FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE
                                                                   595 ANSWERS
100.0% PROCESSED
                      6058 ITERATIONS
SEARCH TIME: 00.00.01
           595 SEA SSS FUL L11
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                STRUCTURE UPLOADED
L1
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25 S L1
L2
L3
            447 S L1 FULL
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L5
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            12 S L4 NOT L5
L6.
             0 S L6 AND DECICCO, C?/AU
L7
             0 S L6 AND HUDYMA, T?/AU
             0 S L6 AND ZHENG, X?/AU
L9
     FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004
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     FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004
L11
               STRUCTURE UPLOADED
L12
            37 S L11
L13
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=> s 113 not 13
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=> file hcaplus
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COST IN U.S. DOLLARS

SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION
ENTRY SESSION

0.00

-9.01

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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CA SUBSCRIBER PRICE

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    FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004
                STRUCTURE UPLOADED
L1
           · 25 S L1
L2
L3
           447 S L1 FULL
     FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004
L4
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L5
             1 S L4 AND PRIESTLEY, E?/AU
            12 S L4 NOT L5
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L11
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L15
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L17
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L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
           Gillio
   Full
         References
                                                                             \mathbf{1}
ACCESSION NUMBER:
                         2003:261620 HCAPLUS
DOCUMENT NUMBER:
                         138:287673
TITLE:
                         Preparation of phenylbenzimidazole compounds useful
                         for treating hepatitis C virus
INVENTOR(S):
                         Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,
                         Thomas W.; Zheng, Xiaofan
                         Bristol-Myers Squibb Company, USA
PATENT ASSIGNEE(S):
                         PCT Int. Appl., 74 pp.
SOURCE:
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
                         English
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                           APPLICATION NO. DATE
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                      KIND DATE
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                                           WO 2002-US30989 20020926
     WO 2003026587
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20031106

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WO 2003026587

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W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
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PRIORITY APPLN. INFO.:
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                                        US 2002-259041
                                                         B1 20020926
OTHER SOURCE(S):
                         MARPAT 138:287673
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Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, AB etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 µM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-49-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN503857-49-6 HCAPLUS

1H-Benzimidazole, 1-cyclohexyl-2-[4-(diphenylmethoxy)phenyl]-5-(1H-CN tetrazol-5-yl) - (9CI) (CA INDEX NAME)

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004 STRUCTURE UPLOADED

L1 STRUC L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED

L12 37 S L11

L13 595 S L11 FULL

L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

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3518 ZHENG, X?/AU

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L18 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing:
Text References
ACCESSION NUMBER:

ACCESSION NUMBER:

AUTHOR(S):

2003:970508 HCAPLUS

OCUMENT NUMBER: 140:174511

TITLE: Mechanism of action and antiviral activity of

benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase

Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini,

Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper, Steven; Stansfield, Ian; Rowley, Michael; De

Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P.

Angeletti", Pomezia-Rome, 00040, Italy

SOURCE: Journal of Virology (2003), 77(24), 13225-13231

CODEN: JOVIAM; ISSN: 0022-538X

PUBLISHER: American Society for Microbiology

DOCUMENT TYPE: Journal LANGUAGE: English

The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the ΑB catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently identified noncatalytic GTP-binding site, thus validating it as a potential allosteric site that can be targeted by small-mol. inhibitors of HCV polymerase.

# IT 658693-60-8

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity);
THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

RN 658693-60-8 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Text References

ACCESSION NUMBER: DOCUMENT NUMBER:

2003:203407 HCAPLUS 138:238181

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

Japan Tobacco Inc., Japan

SOURCE:

GΙ

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PA	PATENT NO.					DATE			A	PPLI	CATIO	ои ис	ο.	DATE			
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		HU,	ID,	IL,	IN,	IS,	KΕ,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
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OTHER SOURCE(S): MARPAT 138:238181									31								

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un) substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1cyclohexylbenzimidazole-5-carboxylate, was given.

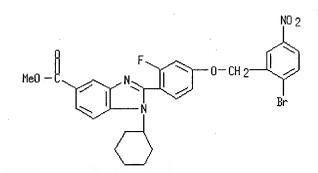
IT 480461-26-5P

CN

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

480461-26-5 HCAPLUS RN

> 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)



Jes Pio isoskro

L18 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Citing References Full Text

ACCESSION NUMBER: 2003:5773 HCAPLUS

138:66657 DOCUMENT NUMBER:

TITLE: Fused cyclic compounds and medicinal use thereof

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, INVENTOR (S):

Patent

Japan Tobacco Inc., Japan PATENT ASSIGNEE(S):

PCT Int. Appl., 603 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE:

Japanese LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PAT	PATENT NO. KIND					DATE			A.	PPLI	CATI	ои ис	Э.	DATE				
									_									
WO	O 2003000254 A1					2003	0103		W	20	02-J	5	20020626					
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US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG JP 2002-185241 JP 2003212846 A2 20030730 20020625 BR 2002005684 Α 20030617 BR 2002-5684 20020626 EP 1400241 20040324 EP 2002-743728 20020626 A1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2003-344997 US 2004082635 A1 20040429 20030218 NO 2003000832 20030422 NO 2003-832 20030221 PRIORITY APPLN. INFO.: A 20010626 JP 2001-193786 JP 2001-351537 A 20011116 WO 2002-JP6405 W 20020626 OTHER SOURCE(S): MARPAT 138:66657

GI

Fused cyclic compds. represented by the following general formula [I] or AΒ pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

## IT 347166-38-5P

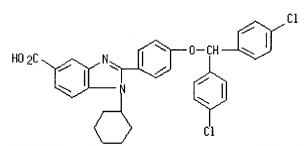
CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

347166-38-5 HCAPLUS RN

> 1H-Benzimidazole-5-carboxylic acid, 2-[4-[bis(4chlorophenyl)methoxy]phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



I

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

27

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Full Citing
Text References
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ACCESSION NUMBER: DOCUMENT NUMBER: 2001:489367 HCAPLUS

TITLE:

Preparation of heterocyclic compounds as remedies for

hepatitis C

135:76874

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

r F

Japan Tobacco Inc., Japan PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

SOURCE:

г. э

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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									JP 2001-193786 A 20010626									

OTHER SOURCE(S):

MARPAT 135:76874

GI

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011  $\mu$ M against hepatitis C virus polymerase. A formulation is given.

### IT 347165-90-6P

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heterocyclic compds. as remedies for hepatitis C)

RN <u>347165-90-6</u> HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 1-cyclopentyl-2-[4-(diphenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

27

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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L8

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0 S L6 AND ZHENG, X?/AU

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STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

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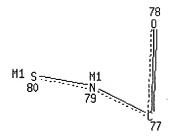
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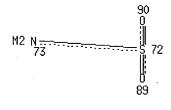
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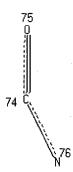
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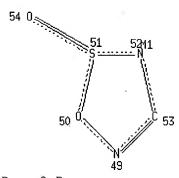




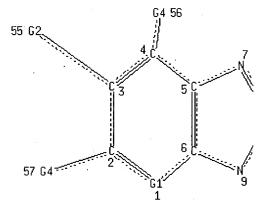
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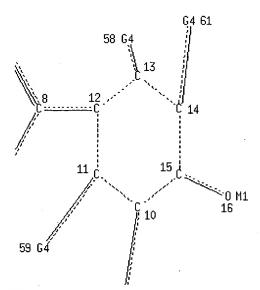


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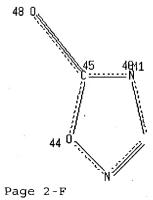


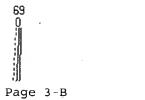
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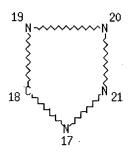
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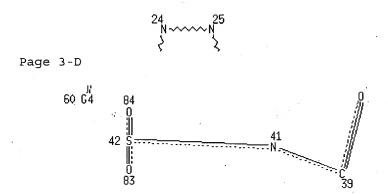




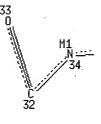
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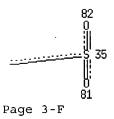
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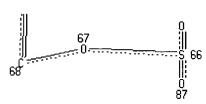


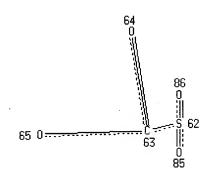












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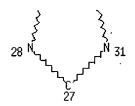
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Page 4-D



Page 4-E

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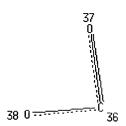
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23



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NSPEC	IS C	AT	74
NSPEC	IS C	AT	75
NSPEC	IS C	AT	76
NSPEC	IS C	AT	77
NSPEC	IS C	AT	78
NSPEC	IS C	AT	79
NSPEC	IS C	AT	80
NSPEC NSPEC	IS C	AT	81
NSPEC NSPEC	IS C	AT AT	82
NSPEC NSPEC			
	IS C	AT	83
NSPEC	IS C	TA	84

NSPEC IS C NSPEC IS C AT 86 NSPEC IS C AT87 NSPEC IS C AT88 NSPEC IS C 89 NSPEC IS C ATDEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 16 32 33 34 35 36 37 38 39 40 41 42 48 54 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85

86 87 88 89 90 93 94 95 96 97 98

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 10 8 43 49 NUMBER OF NODES IS 98

STEREO ATTRIBUTES: NONE

=> s 124

SAMPLE SEARCH INITIATED 01:11:27 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 303 TO ITERATE

100.0% PROCESSED 303 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5016 TO 7104

PROJECTED ANSWERS:

1 TO 80

L25 1 SEA SSS SAM L24

=> s 124 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y FULL SEARCH INITIATED 01:11:34 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 6201 TO ITERATE

100.0% PROCESSED 6201 ITERATIONS

18 ANSWERS

SEARCH TIME: 00.00.01

18 SEA SSS FUL L24 L26

=> file reg

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 166.76 605.98

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) TOTAL SINCE FILE ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -12.48

FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9 DICTIONARY FILE UPDATES: 10 MAY 2004 HIGHEST RN 681120-30-9

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

### => s 126/thu

'THU' IS NOT A VALID CROSSOVER QUALIFIER FOR L26
Answer sets created in a different file may be field qualified with a limited set of qualifiers. Enter <a href="https://example.com/hetp-crossover">HELP CROSSOVER</a> at an arrow prompt (=>) for specific information.

=>	Ιı	ле	ncap.	Lus
COS	T	IN	U.S.	DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.42 606.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE

0.00 -12.48

FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004
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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

### => d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004 L1 STRUCTURE UPLOADED

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L2
            25 S L1
            447 S L1 FULL
L3
     FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004
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L4
             1 S L4 AND PRIESTLEY, E?/AU
L5
             12 S L4 NOT L5
L6
              0 S L6 AND DECICCO, C?/AU
L7
              0 S L6 AND HUDYMA, T?/AU
^{L8}
             0 S L6 AND ZHENG, X?/AU
L9
     FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004
      0 S L3
L10
     FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004
               STRUCTURE UPLOADED
L11
             37 S L11
L12
            595 S L11 FULL
L13
            148 S L13 NOT L3
L14
     FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004
              5 S L14/THU
L15
L16
              1 S L15 AND PRIESTLEY, E?/AU
              0 S L16 NOT L5
L17
L18
              4 S L15 NOT L16
              1 S L15 AND DECICCO, C?/AU
L19
              0 S L19 NOT L16
L20
L21
              0 S L18 AND HYDYMA, T?/AU
L22
              0 S L18 AND ZHENG, X?/AU
     FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004
              0 S L14
L23
     FILE 'REGISTRY' ENTERED AT 00:54:59 ON 12 MAY 2004.
              STRUCTURE UPLOADED
L24
L25
              1 S L24
             18 S L24 FULL
L26
     FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004
     FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004
=> s 126/thu
             8 L26
        591649 THU/RL
             3 L26/THU
L27
                 (L26 (L) THU/RL)
=> d 127, ibib abs fhitstr, 1-3
L27 ANSWER 1 OF 3 HCAPLUS, COPYRIGHT 2004 ACS on STN
                         2003:633749 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         139:180347
                         Preparation of histogranin-like peptides and
TITLE:
                         non-peptides
                         Lemaire, Simon; Bernatchez-Lemaire, Irma; Le,
INVENTOR(S):
                         Hoang-Tanh
```

University of Ottawa, Can.

PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO. KIND DATE
                                           APPLICATION NO. DATE
     _____

        WO
        2003066673
        A1
        20030814

        WO
        2003066673
        C1
        20031204

                                            WO 2003-CA148 20030205
                              20030814
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
              PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
              UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD,
              RU, TJ, TM
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              CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
              NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW,
              ML, MR, NE, SN, TD, TG
     US 2003176329 A1 20030918
                                              US 2002-68905
                                                              20020207
PRIORITY APPLN. INFO.: US
OTHER SOURCE(S): MARPAT 139:180347
                                           US 2002-68905 A 20020207
GΙ
```

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The invention relates to new basic amino acid derivs. I, II and III [A is H, alkyl, or hydroxyalkyl; B is guanidinoalkyl, 4-imidazolylalkyl, aminoalkyl, p-aminophenylalkyl, p-guanidinophenylalkyl, or 4-pyridinylalkyl; D is CO, CO-alkylene, or alkylene; E is a single bond or alkylene; Z is NH2, amino groups, OH, alkoxy, benzyloxy, or halobenzyl; R1-R5 are independently H or various substituents] and to their prepn. and use in treatment of pain. The compds. have histogranin-like antinociceptive, morphine potentiating and COX-2 induction modulating activities. Thus, cyclo[Gly-(p-chloro)Phe-Tyr-D-Arg] (I-1) was prepd. on an oxime resin using tert-butoxycarbonyl (Boc) protection and cleaved from the resin using intrachain aminolysis in the presence of AcOH and diisopropylethylamine. I-1 showed AD50 = 0.17 nmol/mouse and an analgesic potency ratio of 135 relative to histogranin in a mouse writhing pain assay.

# IT 573720-54-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of histogranin-like peptides and non-peptides)

RN 573720-54-4 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-[(1R)-1-(aminocarbonyl)-4-[(aminoiminomethyl)amino]butyl]-2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

2

Full Citing Text References

ACCESSION NUMBER:

2003:203407 HCAPLUS

DOCUMENT NUMBER:

138:238181

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

INVENTOR (S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

Japan Tobacco Inc., Japan

SOURCE:

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

GΙ

Patent

English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT	NO.		KIND	DATE			APPLICATION N					DATE			
							-								
<u>US 2003</u>	05032	0	A1	2003	0313		U	S 20	01-9	39374	1	2001	0824		
WO 2001	047883	3	A1	2001	0705		W	0 20	00-J	P918:	1	2000	1222		
W:	AE,	AG, A	L, AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	CR,	CU, C	Z, DE	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
	HU,	ID, I	L, IN	IS,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
	MA, I	MD, M	G, MK	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
	SG,	SI, S	K, SL	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	YU,	ZA,
	ZW,	AM, A	Z, BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM						
RW:	GH, (	GM, K	E, LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,
	DE, I	DK, E	S, FI	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
	ВJ, (	CF, C	G, CI,	CM,	GΑ,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
JP 2001	24755	0	A2	2001	0911		J.	P 20	00-3	91904	1	2000	1225		
PRIORITY APP	LN. II	NFO.:					JP 1	999-	3690	8 0	A	1999	1227		
						1	WO 2	000-	JP91	81	A2	2000	1222		
						i	JP 2	000-	3919	04	A	2000	1225		
							JP 2	001-	1937	86	Α	2001	0626		
OTHER SOURCE	(S):		MAI	RPAT	138::	2381	81								

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5,

G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un) substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1cyclohexylbenzimidazole-5-carboxylate, was given.

# IT 347165-36-0P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN347165-36-0 HCAPLUS

> 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-(4-hydroxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

L27 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

Text References

ACCESSION NUMBER:

2001:489367 HCAPLUS

DOCUMENT NUMBER:

TITLE:

135:76874

Preparation of heterocyclic compounds as remedies for hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

SOURCE:

Japan Tobacco Inc., Japan

PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	NO.		ΚI	ND	DATE			A	PPLI	CATI	ON NO	o. :	DATE			
								_						<i>-</i>		
WO 200	10478	83	Α	1	2001	0705		W	O 20	00-J	P918	1	2000	1222		
W:	ΑE,	AG,	AL,	AM,	ΑT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,
	HU,	ID,	ΙL,	IN,	IS,	ΚE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
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	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,
	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
EP 116	2196		Α	1	2001	1212		E	P 20	00-9	8772	8	2000	1222		
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	ΙE,	SI,	LT,	LV,	FI,	RO										
BR 200	00085	25	Α		2002	0102		B	R 20	00-8	525		2000	1222		

TR 200	103147	T1	20020621	TR	2001-20010	314	720001222
NZ 514	403	Α	20021025	NZ	2000-51440	3	20001222
AU 763	356	B2	20030717	AU	2001-24017		20001222
RU 222	3761	C2	20040220	RU	2001-12628	3	20001222
NO 200	1004134	A ·	20011022	NO	2001-4134		20010824
<u>US 200</u>	3050320	A1	20030313	US	2001-93937	4	20010824
ZA 200	1007870	A	20020925	ZA	2001-7870		20010928
PRIORITY AF	PLN. INFO.:			JP 19	99-369008	Α	19991227
				WO 20	00-JP9181	M	20001222
				JP 20	00-391904	Α	20001225
				JP 20	01-193786	Α	20010626

OTHER SOURCE(S):

MARPAT 135:76874

GI

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011  $\mu$ M against hepatitis C virus polymerase. A formulation is given.

# IT 347165-36-0P

RN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heterocyclic compds. as remedies for hepatitis C)

347165-36-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-(4-hydroxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

CA SUBSCRIBER PRICE

27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

-2.08

-14.56

=> file caold
COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE TOTAL
ENTRY SESSION
ENTRY SESSION

FILE 'CAOLD' ENTERED AT 01:12:49 ON 12 MAY 2004
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REG1STRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

### => d his

L1

L10

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004 STRUCTURE UPLOADED 25 S L1

L2 25 S L1 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU

L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48, ON 12 MAY 2004 0 S L3

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STRUCTURE UPLOADED
L11
L12
            37 S L11
           595 S L11 FULL
L13
           148 S L13 NOT L3
    FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004
     5 S L14/THU
L15
            1 S L15 AND PRIESTLEY, E?/AU
L16
            0 S L16 NOT L5
L17 ·
L18
            4 S L15 NOT L16
            1 S L15 AND DECICCO, C?/AU
L19
            0 S L19 NOT L16
            0 S L18 AND HYDYMA, T?/AU
L21
            0 S L18 AND ZHENG, X?/AU
L22
    FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004
           0 S L14
L23
     FILE 'REGISTRY' ENTERED AT 00:54:59 ON 12 MAY 2004
L24
              STRUCTURE UPLOADED
L25
             1 S L24
            18 S L24 FULL
L26
     FILE 'REGISTRY' ENTERED AT 01:11:38 ON 12 MAY 2004
     FILE 'HCAPLUS' ENTERED AT 01:11:52 ON 12 MAY 2004
L27
             3 S L26/THU
     FILE 'CAOLD' ENTERED AT 01:12:49 ON 12 MAY 2004
=> s 126
L28
            0 L26
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FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

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             39 40 42
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             83
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g nodes :
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in bonds :
2-84 3-66 4-83 9-13 11-86 12-85 14-87 15-88 16-17 17-82 37-38 37-39 39-40 42-43 42-45 46-47 46-48 48-49 53-56 60-63 67-68 70-71 71-72 74-75 75-76 78-79
g bonds:
1-2 1-6 2-3 3-4 4-5 5-6 5-8
15-16 19-20 19-23 20-21 21-22
32-33 33-34 34-35 51-52 51-55
                                                  6-10 8-9 9-10 11-12 11-16 12-13 13-14 14-15 22-23 25-26 25-29 26-27 27-28 28-29 31-32 3 52-53 53-54 54-55 58-59 58-62 59-60 60-61 6
                                                                                                                         31 - 35
          33-34 34-35
ct/norm bonds :
                               3-4 3-66 4-5 4-83 5-6 5-8 6-10 8-9
17-82 19-20 19-23 20-21 21-22 22-23
                                                                                           9-10
25-26
                      2-84
1-2 1-6 2-3
                                                                                                     9-13
                                                                                                             11-86 12-85
14-87
          15-88
                    16-17
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42-45
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51-55
71-72
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 28-29
          31-32
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                                         33-34
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                                                                                 39-40
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74-75
 48-49
           51-52
                                         53-54
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                                                             54-55 58-59 58-62
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 67-68
                                         75-76
          70-71
                                                   78-79
malized bonds :
11-12 11-16
                   12-13 13-14 14-15
                                                  15-16
lated ring systems :
  containing 1 : 11 : 51 : 58 :
C,N
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13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

11:Atom

12:Atom

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom

[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8]

Cy,[\*9],[\*10],[\*11],[\*12]

ch level :

25:Atom

26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS 72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 83:CLASS 84:CLASS 85:CLASS 86:CLASS 87:CLASS 88:CLASS

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ng bonds :
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olated ring systems :
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C,N
[*1],[*2],[*3],[*4],[*5],[*6],[*7],[*8],[*9],[*10]
Cy,[*11],[*12],[*13],[*14]
H,F,CH3,NH2
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ch level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 55:Atom 56:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS 72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS 87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS

#### => d his (FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004) FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004 STRUCTURE UPLOADED L125 S L1 L2L3447 S L1 FULL FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004 L413 S L3 1 S L4 AND PRIESTLEY, E?/AU L5 L6 12 S L4 NOT L5 0 S L6 AND DECICCO, C?/AU L7 0 S L6 AND HUDYMA, T?/AU L80 S L6 AND ZHENG, X?/AU L9 FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004 0 S L3 L10 FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004 STRUCTURE UPLOADED L11 37 S L11 L12595 S L11 FULL L13 148 S L13 NOT L3 L14FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004 L15 5 S L14/THU 1 S L15 AND PRIESTLEY, E?/AU L16 L17 0 S L16 NOT L5 . 4 S L15 NOT L16 L18 1 S L15 AND DECICCO, C?/AU L19 L20 0 S L19 NOT L16 L21 0 S L18 AND HYDYMA, T?/AU L22 0 S L18 AND ZHENG, X?/AU FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004

=> s 114 L23

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NEWS 4	JAN	27	A new search aid, the Company Name Thesaurus, available in CA/CAplus
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			available
NEWS 14			LITALERT now available on STN
NEWS 15			NLDB: New search and display fields available PROUSDDR now available on STN
NEWS 16	_		PROUSDDR: One FREE connect hour, per account, in both May
NEWS 17	May	10	and June 2004
NEWS EXP	RESS	MA	RCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), D CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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FULL ESTIMATED COST

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L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS L1 ST

=> s 11 SAMPLE SEARCH INITIATED 00:32:07 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE

100.0% PROCESSED 302 ITERATIONS SEARCH TIME: 00.00.01

25 ANSWERS

DIARCH TIME. 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*
BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 4998 TO 7082
PROJECTED ANSWERS: 200 TO 800

L2 25 SEA SSS SAM L1

=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 00:32:12 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE

100.0% PROCESSED 6058 ITERATIONS 447 ANSWERS SEARCH TIME: 00.00.01

L3 447 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

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FULL ESTIMATED COST

168.44

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 13 L3

=> s l4 and priestley, e?/au 64 PRIESTLEY, E?/AU

L5 1 L4 AND PRIESTLEY, E?/AU

=> d 15, ibib abs fhitstr, 1

L5 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing Text References

ACCESSION NUMBER: 2003:261620 HCAPLUS

DOCUMENT NUMBER: 138:287673

TITLE: Preparation of phenylbenzimidazole compounds useful

for treating hepatitis C virus

INVENTOR(S): Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,

Thomas W.; Zheng, Xiaofan

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT I	NO.		KII	ND	DATE			A	PPLI	CATIO	ON NO	o. :	DATE				
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	WO 2003	0265	<u>87</u>	A:	2	2003	0403		W	20	02-U	53098	39	2002	0926			
	WO 2003	0265	87	A.	3	2003	1106											
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		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
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Me	US 2003	1348	53	A:	1.	2003	0717		<u>U:</u>	S 20	02-2	5904	1	2002	0926			
8	US 2004	0679	76	A:	1	2004	0408		<u>U:</u>	S 20	03-6	1887	3_	2003	0827			
PRIORITY APPLN. INFO.:								ļ	US 2	001-	3248	74P	P	2001	0926			
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http://stnweb.cas.org/cgi-bin/sdcgi?SID=584392-1745035756-200&APP=stnweb&

US 2002-259041 B1 20020926

OTHER SOURCE(S): MARPAT 138:287673

Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14  $\mu$ M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

RN 503857-56-5 HCAPLUS

Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-yl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 503857-55-4 CMF C40 H41 N7 O5 S

CM 2

CRN  $\frac{76-05-1}{C2 H F3}$  O2

=> d his

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004

STRUCTURE UPLOADED L1

25 S L1 L2

447 S L1 FULL L3

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

13 S L3 L4

1 S L4 AND PRIESTLEY, E?/AU L5

=> s 14 not 15

12 L4 NOT L5

=> s 16 and decicco, c?/au

125 DECICCO, C?/AU

0 L6 AND DECICCO, C?/AU

=> s 16 and hudyma, t?/au

45 HUDYMA, T?/AU

0 L6 AND HUDYMA, T?/AU

=> s 16 and zheng, x?/au

3518 ZHENG, X?/AU

0 L6 AND ZHENG, X?/AU

=> d 16, ibib abs fhitstr, 1-12

ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN L6

(Cielale) References Text ACCESSION NUMBER:

2003:981461 HCAPLUS

DOCUMENT NUMBER:

140:246106

TITLE:

Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of

benzimidazole derivatives

AUTHOR (S):

Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet,

Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin,

Charles; Austel, Volkhard; Kukolj, George

CORPORATE SOURCE:

Department of Chemistry, Research and Development, Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S

2G5, Can.

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2004),

14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Benzimidazole 5-carboxamide derivs. from a combinatorial screening library AB were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

## IT 390815-16-4P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

390815-16-4 HCAPLUS RN

> 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN L6

(cliffie) References

ACCESSION NUMBER: DOCUMENT NUMBER:

2003:319709 HCAPLUS

138:338144

TITLE:

Maybe: mhe sine Them Preparation of 2-phenyl benzimidazoles and

imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the

treatment of cancer

Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J. INVENTOR(S):

Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.

Ortho-McNeil Pharmaceutical, Inc., USA PATENT ASSIGNEE(S): PCT Int. Appl., 144 pp.

Patent

SOURCE: CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

107Ce provision

		7
JICATION NO.	DATE	0
2002-US33371	20021018	

PATENT NO. APPL KIND DATE ----\_ \_ \_ \_ WO 2003032984 20030424 WO 2 A1 WO 2003032984 C1 20031120 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,

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PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
                            20030918
                                            US 2002-273487
                                                             20021018
    US 2003176438
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                                            NO 2003-2759
                            20030818
                                                             20030617
     NO 2003002759
                       Α
                                        US 2001-330304P
PRIORITY APPLN. INFO.:
                                                          Ρ
                                                             20011019
                                        WO 2002-US33371
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OTHER SOURCE(S):

MARPAT 138:338144

GΙ

$$\begin{array}{c} \text{N} \\ \text{N} \\ \text{R?} \\ \text{R?} \end{array} \begin{array}{c} \text{N} \\ \text{NH} \\ \text{NH} \end{array} \begin{array}{c} \text{Y=Y-Ar 1} \\ \text{Y1-Y2} \\ \text{I} \end{array}$$

2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; e.g. 2-[4-(4-chlorophenoxy) phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cdsl and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(0)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1 or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Arl is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide. Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example prepns. are included.

IT 516480-80-1P, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5-

carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

RN 516480-80-1 HCAPLUS

CN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2004 ACS on STN L6 ANSWER 3 OF 12

ACCESSION NUMBER:

2003:203407 HCAPLUS

DOCUMENT NUMBER:

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

138:238181

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

SOURCE:

Japan Tobacco Inc., Japan

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT 1	NO.		KII	1D	DATE			A	PPLI	CATI	ои ис	<b>).</b> , !	DATE			
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US 2003	0503	20 -	A.	1 :	2003	0313		<u>U</u> :	S 20	01-9	3937	4	2001	0824		
WO 2001	0478	83	A.	1	2001	0705		W	200	00-J	P918	1	2000	1222		
W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
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JP 2001247550 PRIORITY APPLN. INFO.:

JP 2000-391904 20001225 A 19991227 JP 1999-369008

A2 20001222 WO 2000-JP9181 JP 2000-391904 A 20001225

JP 2001-193786 A 20010626

OTHER SOURCE(S):

MARPAT 138:238181

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The title compds. I [the dotted line in rings B1 and B2 indicates a single AB or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy =(un) substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data

given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1cyclohexylbenzimidazole-5-carboxylate, was given.

IT 347165-35-9P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

347165-35-9 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1cyclohexyl- (9CI) (CA INDEX NAME)

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References Text

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

INVENTOR (S):

2003:5773 HCAPLUS

138:66657 Fused cyclic compounds and medicinal use thereof

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

PATENT ASSIGNEE(S):

SOURCE:

Japan Tobacco Inc., Japan PCT Int. Appl., 603 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent

Japanese FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PAT	CENT 1	NO.		KII	ND :	DATE			Al	PLI	CATIO	ои ис	<b>).</b> 1	DATE			
	WO	2003	0002	54	<b>A</b> :	 1	2003	0103		W(	20	02-J	P640!	5	2002	0626		
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PRIORITY APPLN. INFO.:

 JP 2001-193786
 A 20010626

 JP 2001-351537
 A 20011116

 WO 2002-JP6405
 W 20020626

OTHER SOURCE(S):

MARPAT 138:66657

GΙ

I

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

IT 347165-35-9P

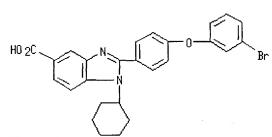
CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347165-35-9 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

DOCUMENT NUMBER:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

27

Full Citing.
Text References.
ACCESSION NUMBER:

2002:51438 HCAPLUS

136:118447

TITLE: Preparation of benzimidazolecarboxylates and related

compounds as viral polymerase inhibitors

INVENTOR(S): Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James;

Kukolj, George; Austel, Volkhard

PATENT ASSIGNEE(S): Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE: PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

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LANGUAGE:
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
          PATENT NO.
          WQ 2002004425
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 PRIORITY APPLN. INFO.:
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                                                                                <u>US 2001-281343P</u>
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                                                                                US 2001-995099
                                                                                                                  A3 20011127
                                                                                 WO 2002-CA323
                                                                                                                  W 20020306
                                                  MARPAT 136:118447
 OTHER SOURCE(S):
 GΙ
                               (CH 2)nCYZ
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Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH2, NMeR3, NHR3, OR3, S-6AB membered (substituted) heterocyclyl; A = N, COR7, CR5; R5 = H, halo, alkyl; R7 = H, alkyl; X and A are not both N; R6 = H, halo, alkyl, OR7; R7 = H , alkyl; R1 = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF3; R2 = (substituted) alkyl,

cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5 µM.

## IT 347166-09-0P

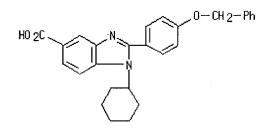
CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN 347166-09-0 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Citing
Text References

SOURCE:

ACCESSION NUMBER: 2001:489367 HCAPLUS

DOCUMENT NUMBER: 135:76874

TITLE: Preparation of heterocyclic compounds as remedies for

hepatitis C

INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan

PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2001047883 A1 20010705 WO 2000-JP9181 20001222 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR; BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG EP 1162196 A1 20011212 EP 2000-987728

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NO 20010	04134	A		2001	1022		NO	200	01-4	134		2001	0824		
<u>US 20030</u>	50320	A	1.	2003	0313		<u>U</u> :	S 200	01-9	3937	4 :	2001	0824		
ZA 20010	07870	Α		2002	0925		$\mathbf{Z}_{\mathbf{Z}}$	A 200	01-7	870	:	2001	0928		
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							WO 2	000-	JP91	81	W	2000	1222		
							JP 2	000-3	3919	04	Α :	2000	1225		
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OTHER SOURCE(S):

MARPAT 135:76874

GΙ

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 $G_{2}^{61}G_{1}^{68}G_{1}^{67}G_{1}^{66}$ 
 $G_{3}^{64}G_{1}^{69}G_{1}^{65}G_{1}^{65}$ 
 $G_{4}^{66}G_{1}^{69}G_{1}^{69}G_{1}^{66}G_{1}^$ 

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μM against hepatitis C virus polymerase. A formulation is given.

Π

# IT 347165-35-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heterocyclic compds. as remedies for hepatitis C)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)

HO 2C

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 **HCAPLUS** COPYRIGHT 2004 ACS on STN ANSWER 7 OF 12

27

ACCESSION NUMBER:

TITLE:

DOCUMENT NUMBER:

135:177890 Synthesis and antimicrobial activity of some new

2-phenyl-N-substituted carboxamido-1H-benzimidazole

derivatives

AUTHOR (S):

Goker, Hakan; Tuncbilek, Meral; Suzen, Sibel; Kus,

Canan; Altanlar, Nurten

Wiley-VCH Verlag GmbH

2001:412102 HCAPLUS

CORPORATE SOURCE:

Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University, Ankara, 06100, Turk.

SOURCE:

Archiv der Pharmazie (Weinheim, Germany) (2001

334(5), 148-152 CODEN: ARPMAS; ISSN: 0365-6233

Journal

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

English CASREACT 135:177890

NH CH 2CH 2NMe 2

NH CH 2CH 2NEt 2

NH CH 2CH 2NMe 2 F 3C

AB Some 1H-benzimidazole-carboxamide derivs. were prepd. and their antimicrobial activities against Staphylococcus aureus, Escherichia coli,

III

and Candida albicans evaluated. Compds. I, II, and III exhibited the best activity against C. albicans.

IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and antimicrobial activity of new 2-phenyl-N-substituted carboxamido-1H-benzimidazole derivs.)

174422-18-5 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) CN (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

COPYRIGHT 2004 ACS on STN HCAPLUS L6 ANSWER 8 OF 12

8

Text

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

AUTHOR (S):

CORPORATE SOURCE:

SOURCE:

PUBLISHER: DOCUMENT TYPE:

LANGUAGE:

GT

1999:614608 HCAPLUS

131:286454

Synthesis and antimicrobial activity of some new

benzimidazole carboxylates and carboxamides

Ayhan-Kilcigil, Gulgun; Tuncbilek, Meral; Altanlar,

Nurten; Goker, Hakan

Department of Pharmaceutical Chemistry, Faculty of

Pharmacy, Ankara University, Ankara, 06100, Turk.

Farmaco (1999), 54(8), 562-565 CODEN: FRMCE8; ISSN: 0014-827X

Elsevier Science S.A.

Journal English

AB Benzimidazole carboxylates and carboxamides, e.g., I [R1 = MeO, (2-pyridinylmethyl)amino, 4-methylpiperidino, R2 = 2-ClC6H4, 4-ClC6H4, 2,4-Cl2C6H3, 2-MeOC6H4, 4-MeOC6H4, 2-thienyl], were synthesized and evaluated for their antimicrobial activities against Staphylococcus aureus, Escherichia coli, and Candida albicans. Among the investigated compds., I (R1 = MeO, R2 = 2-MeOC6H4) exhibited best activity against C. albicans.

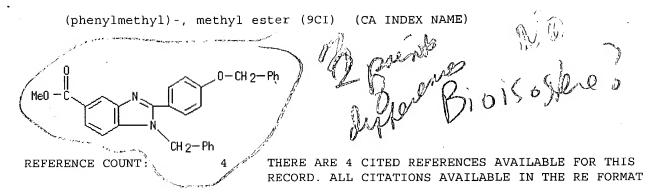
IT 246517-85-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and antimicrobial activity of benzimidazole carboxylates and carboxamides)

246517-85-1 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]-1-CN



L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

# Full Citing Text References

ACCESSION NUMBER:

1999:184240 HCAPLUS 130:209707

DOCUMENT NUMBER: TITLE:

Preparation of 2-substituted phenyl-benzimidazole

antibacterial agents

INVENTOR(S):

Ohemeng, Kwasi Adomako; Nguyen, Van Nhatton Ortho-McNeil Pharmaceutical, Inc., USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 70 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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			LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,		
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	UA,	UG,	UZ,		
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		-								WO 1	998-	US18	<u> 586</u>		1998	0904			$\mathcal{L}$	/

OTHER SOURCE(S):

MARPAT 130:209707

GI

$$R^{5}$$
 $R^{7}$ 
 $R^{1}$ 
 $R^{2}$ 
 $R^{3}$ 

AB Benzimidazoles I [R1 = H, OH, alkoxy; R2, R3, R4 = H, OH, alkyl, CF3, halo, etc.; R5 = H, amino, amidino; R6 = nitro, C(NHR9):NR10; R7 = H, amino, nitro; R8 = H, Me], antibacterial compds., were prepd. These compds. are effective in inhibiting the action of a bacterial histidine protein kinase and are useful as anti-infective agents against a variety

of bacterial organisms, including organisms which are resistant to other known antibiotics. E.g., 3,4-diaminobenzimidate, prepd. from 3,4-diaminobenzonitrile, was treated with NH3/EtOH, then with 4-Me3CC6H4CHO to give 2-[4-(1,1-dimethylethyl)phenyl]-2H-benzimidazole-5-carboximidamide.

### IT 220955-73-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of phenylbenzimidazoles as antibacterial agents)

RN 220955-73-7 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-(4-phenoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER: 1998:634393 HCAPLUS

DOCUMENT NUMBER: 129:316174

TITLE: Synthesis of some new benzimidazolecarboxamides and

evaluation of their antimicrobial activity

AUTHOR(S): Goker, Hakan; Tuncbilek, Meral; Ayhan, Gulgun;

Altanlar, Nurten

CORPORATE SOURCE: Department of Pharmaceutical Chemistry, Faculty of

Pharmacy, Ankara University, Ankara, 06100, Turk.

SOURCE: Farmaco (1998), 53(6), 415-420

CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Elsevier Science S.A.

DOCUMENT TYPE: Journal LANGUAGE: English

AB A series of 1,2-disubstituted benzimidazole-5(6)-carboxamides was prepd. and evaluated in vitro for antimicrobial activity against Staphylococcus aureus, Escherichia coli, and Candida albicans. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids with aldehydes and via several steps over the 2(1H)-benzimidazolones, resp. All acids were converted to their acyl chlorides with SOC12, then amidified with several N,N'-dialkylaminoethyl derivs.

# IT 174422-18-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (prepn. and bactericidal and fungicidal activity of
 benzimidazolecarboxamides)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI)
(CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Claing Text References

ACCESSION NUMBER:

1996:144268 HCAPLUS

DOCUMENT NUMBER:

124:197998

TITLE:

Synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial

activity

AUTHOR (S):

Goeker, Hakan; Tebrizli, Emin; Abbasoglu, Ufuk

CORPORATE SOURCE:

Faculty of Pharmacy, Univ. of Ankara, Tandogan, 06100,

Turk

SOURCE:

Farmaco (1996), 51(1), 53-8

CODEN: FRMCE8

PUBLISHER:

Societa Chimica Italiana

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Fourteen N'-(N,N-dialkylaminoethyl)-benzimidazole 5(6)- or 5-carboxamides having several substituents on the azole and benzene nuclei were prepd. and evaluated in vitro for antimicrobial activity. The precursor benzimidazolecarboxylic acids were prepd. via oxidative condensation of diaminobenzoic acids and several aldehydes with cupric ion. All carboxamides were prepd. from the corresponding acids and N,N-dialkylethylenediamine. Antibacterial and antifungal activities were detd. as MIC values. Compds. which were prepd. by replacement with bulky alkyl groups on the tert-N benzimidazole atom gave the best results.

IT 174422-18-5P

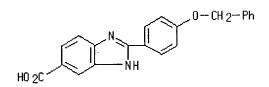
RL: PRP (Properties); PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (synthesis of 1,2-disubstituted benzimidazole-5(6)-carboxamides and evaluation of their antimicrobial activity)

RN 174422-18-5 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

(OII INDEN MAID)





L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN



ACCESSION NUMBER:

1996:38013 HCAPLUS

DOCUMENT NUMBER:

124:202112

TITLE:

CN

Synthesis of some new benzimidazole-5(6)-carboxylic

acids

AUTHOR (S):

Goeker, Hakan; Oelgen, Suereyya; Ertan, Rahmiye;

Akguen, Huelya; Oezbey, Sueheyla; Kendi, Engin; Topcu,

Guel

CORPORATE SOURCE:

SOURCE:

Fac. Pharmacy, Ankara Univ., Ankara, 06100, Turk.

Journal of Heterocyclic Chemistry (1995), 32(6),

1767-73

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER:

DOCUMENT TYPE:

LANGUAGE:

Journal

HeteroCorporation

English

GΙ

The title compds., 1,2-dialkyl-benzimidazole-5(6)-carboxylic acids I (Ar = Ph, 4-MeC6H4, 4-ClC6H4, 2-BrC6H4, OPh, 4-ClC6H4O, etc., R = H, F, CO2H position = 5, 6) were prepd. in four steps; (1) prepn. of mono amide derivs. II by the reaction of Me 3,4-diaminobenzoate and substituted Ph or phenoxyacetic acid chlorides ArCH2COCl, (2) prepn. of the Me benzimidazolecarboxylates III, with zinc chloride and dry hydrogen chloride gas, (3) alk. hydrolysis of the esters, and (4) substitution of the imidazole ring with benzyl or p-fluorobenzyl bromide, in alkali medium. 2-Aryl-benzimidazole-5(6)-carboxylic acids IV (R1 = H, OCH2Ph, OH, R2 = OCH2Ph, OH) were prepd. via the oxidative condensation of 3,4-diaminobenzoic acid and arom. aldehydes with cupric ion.

## IT 174422-18-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazolecarboxylic acids)

RN 174422-18-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

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L1 STRUCTURE UPLOADED

L2 25 S L1 L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU

L8 0 S L6 AND HUDYMA, T?/AU

L9 0 S L6 AND ZHENG, X?/AU

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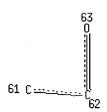
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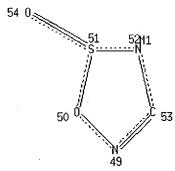
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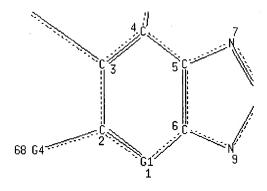
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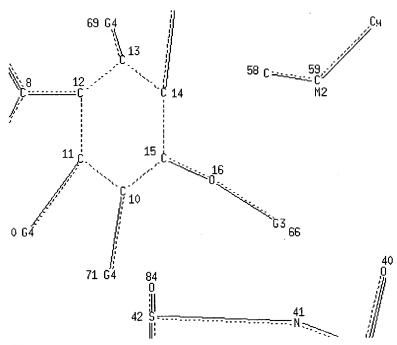
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Page 2-A

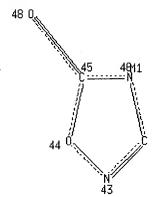


Page 2-B

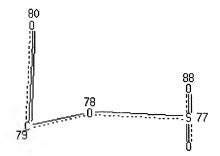




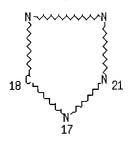
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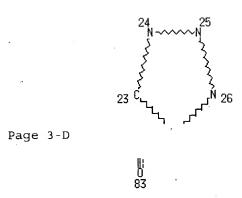


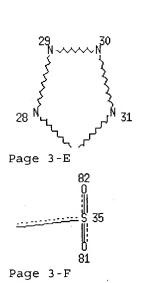
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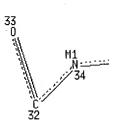


Page 3-B

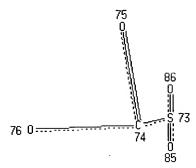








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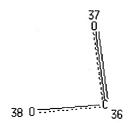


Page 4-B



Page 4-D

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Page 4-E

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VAR G3=91/57/58/61/64

VAR G4=92/93/94/95

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THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
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FULL SEARCH INITIATED 00:47:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE
100.0% PROCESSED
                   6058 ITERATIONS
                                                           595 ANSWERS
SEARCH TIME: 00.00.01
           595 SEA SSS FUL L11
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     (FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)
     FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004
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STRUCTURE UPLOADED

L1

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L2
             25 S L1
L3
            447 S L1 FULL
     FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004
             13 S L3
L4
             1 S L4 AND PRIESTLEY, E?/AU
L5
             12 S L4 NOT L5
L6
              0 S L6 AND DECICCO, C?/AU
L7
              0 S L6 AND HUDYMA, T?/AU
L8
              0 S L6 AND ZHENG, X?/AU
Ь9
     FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004
              0 S L3
L10
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                STRUCTURE UPLOADED
L11
             37 S L11
L12
            595 S L11 FULL
L13
=> s 113 not 13
       148 L13 NOT L3
=> file hcaplus
COST IN U.S. DOLLARS
                                                  SINCE FILE
                                                                  TOTAL
                                                       ENTRY
                                                                SESSION
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FULL ESTIMATED COST
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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
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FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004
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ENTRY

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SESSION

-9.01

FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 10 May 2004 (20040510/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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5 Ll4

591649 THU/RL

Ll5 5 Ll4/THU

(Ll4 (L) THU/RL)
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CA SUBSCRIBER PRICE

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L16
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L2
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L3
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     FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004
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L5
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L10
     FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004
                STRUCTURE UPLOADED
L11
             37 S L11
L12
L13
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            148 S L13 NOT L3
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L15
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L16 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN
         Citing
References
                         2003:261620 HCAPLUS
ACCESSION NUMBER:
DOCUMENT NUMBER:
                         138:287673
                         Preparation of phenylbenzimidazole compounds useful
TITLE:
                         for treating hepatitis C virus
                         Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,
INVENTOR(S):
                         Thomas W.; Zheng, Xiaofan
                         Bristol-Myers Squibb Company, USA
PATENT ASSIGNEE(S):
SOURCE:
                         PCT Int. Appl., 74 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
                         English
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                           APPLICATION NO. DATE
     PATENT NO.
                      KIND DATE
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                            20030403
                                           WO 2002-US30989 20020926
     WO 2003026587
                       A2
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20031106

A3

WO 2003026587

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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
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             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
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                                           US 2002-259041
                                                            20020926
     US 2004067976 🥆
                       A1
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                                                            20030827
PRIORITY APPLN. INFO
                                        US 2001-324874P
                                                            20010926
                                        US 2002-259041
                                                         B1 20020926
OTHER SOURCE(S):
                         MARPAT 138:287673
GI
                                                                  1725904/
                                        Π
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AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 µM against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-49-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of phenylbenzimidazole compds. for treating hepatitis  ${\tt C}$  viral infection)

RN 503857-49-6 HCAPLUS

CN 1H-Benzimidazole, 1-cyclohexyl-2-[4-(diphenylmethoxy)phenyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)

=> d his

L1

(FILE 'HOME' ENTERED AT 00:12:55 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 00:13:07 ON 12 MAY 2004 STRUCTURE UPLOADED

L2 25 S L1

L3 447 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 00:32:16 ON 12 MAY 2004

L4 13 S L3

L5 1 S L4 AND PRIESTLEY, E?/AU

L6 12 S L4 NOT L5

L7 0 S L6 AND DECICCO, C?/AU
L8 0 S L6 AND HUDYMA, T?/AU
L9 0 S L6 AND ZHENG, X?/AU

FILE 'CAOLD' ENTERED AT 00:33:48 ON 12 MAY 2004

L10 0 S L3

FILE 'REGISTRY' ENTERED AT 00:33:56 ON 12 MAY 2004

L11 STRUCTURE UPLOADED

L12 37 S L11

L13 595 S L11 FULL L14 148 S L13 NOT L3

FILE 'HCAPLUS' ENTERED AT 00:47:52 ON 12 MAY 2004

L15 5 S L14/THU

L16 1 S L15 AND PRIESTLEY, E?/AU

L17 0 S L16 NOT L5

=> s 115 not 116

L18 4 L15 NOT L16

=> s 115 and decicco, c?/au

125 DECICCO, C?/AU

L19 1 L15 AND DECICCO, C?/AU

=> s 119 not 116

L20 0 L19 NOT L16

=> s 118 and hydyma, t?/au

O HYDYMA, T?/AU

L21 0 L18 AND HYDYMA, T?/AU

=> s 118 and zheng, x?/au

3518 ZHENG, X?/AU

L22 0 L18 AND ZHENG, X?/AU

### => d l18, ibib abs fhitstr, 1-4

ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text

ACCESSION NUMBER:

2003:970508 HCAPLUS 140:174511

DOCUMENT NUMBER:

TITLE:

AUTHOR (S):

Mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini, Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper,

Steven; Stansfield, Ian; Rowley, Michael; De Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE:

Istituto di Ricerche di Biologia Molecolare "P.

Angeletti", Pomezia-Rome, 00040, Italy

SOURCE:

Journal of Virology (2003), 77(24), 13225-13231

CODEN: JOVIAM; ISSN: 0022-538X American Society for Microbiology

DOCUMENT TYPE:

PUBLISHER:

Journal English

LANGUAGE:

The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently

IT 658693-60-8

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

identified noncatalytic GTP-binding site, thus validating it as a

potential allosteric site that can be targeted by small-mol. inhibitors of

658693-60-8 HCAPLUS RN

HCV polymerase.

1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-CN piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1cyclohexyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

HCAPLUS COPYRIGHT 2004 ACS on STN L18 ANSWER 2 OF 4

ACCESSION NUMBER:

2003:203407 HCAPLUS

DOCUMENT NUMBER:

138:238181

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

Japan Tobacco Inc., Japan

SOURCE:

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT	KI	KIND DATE				Al	PPLI	CATI	ои ис	Ο.	DATE							
US 2003	US 2003050320			A1 20030313			US 2001-939374					20010824						
WO 2001	WO 2001047883			20010705			WO 2000-JP9181					20001222						
-			_								-							
₩:	AE,	AG, AL,	AM,	AΤ,	ΑU,	AZ,	BA,	BB,	ВG,	BR,	BY,	BZ,	CA,	CH,	CN,			
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	HU,	ID, IL,	IN,	IS,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,			
	MA,	MD, MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,			
	SG,	SI, SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VN,	YU,	ZA,			
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RW:	GH,	GM, KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,			
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JP 2001	24755	0 A	.2 2	2001	0911		J	20	00-3	91904	1	2000	1225					
PRIORITY APP	LN. I	NFO.:				١	ĴΡ 19	999-	3690	<u>8</u>	Α	1999	1227					
						1	WO 20	000-	JP91	81	A2	2000	1222					
						1	JP 20	000-	3919	04	Α	2000	1225					
							JP 20	001-	1937	86	Α	2001	0626					
OTHER SOURCE	(8) .		MARI	ייעם	138.1	2381	81											

OTHER SOURCE(S):

MARPAT 138:238181

GΙ

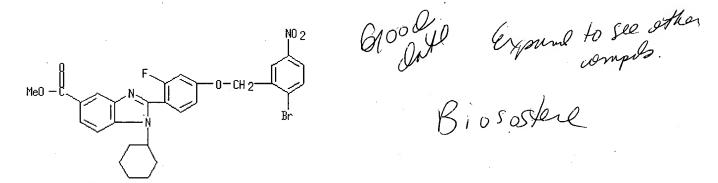
- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1-cyclohexylbenzimidazole-5-carboxylate, was given.

### IT 480461-26-5P

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

RN 480461-26-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)



L18 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

Text References

ACCESSION NUMBER:

2003:5773 HCAPLUS

DOCUMENT NUMBER:

138:66657

TITLE:

Fused cyclic compounds and medicinal use thereof

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S): SOURCE:

Japan Tobacco Inc., Japan PCT Int. Appl., 603 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

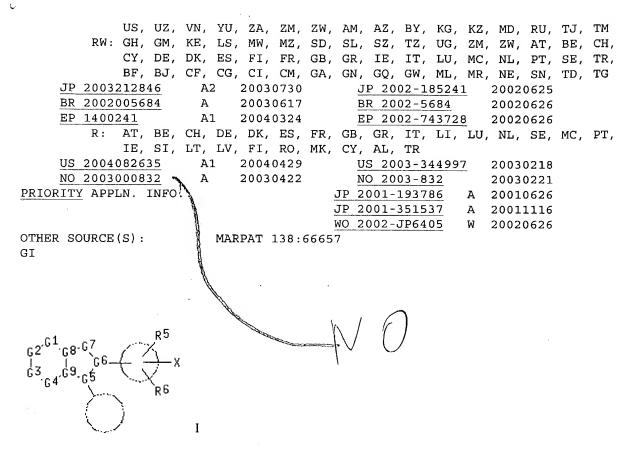
Japanese

FAMILY ACC. NUM. COUNT:

: 3

PATENT INFORMATION:

PATENT NO. KIND						ND :	DATE			A.	PPLI	CATIO	ои ис	٥.	DATE			
						-, -				-								
	WO	2003	0002	54	A:	1	2003	0103		W	20	02-J	P640	5	2002	0626		
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	ĢΕ,	GH,
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			RO.	RU.	SD.	SE.	SG.	SI.	SK.	SL.	TJ.	TM.	TN.	TR.	TT.	TZ.	IJA.	UG.



AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

IT 347166-38-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347166-38-5 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-[bis(4-chlorophenyl)methoxy]phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2004 ACS on STN

27

ACCESSION NUMBER:

2001:489367 HCAPLUS

DOCUMENT NUMBER:

135:76874

TITLE:

Preparation of heterocyclic compounds as remedies for

hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S): SOURCE:

Japan Tobacco Inc., Japan PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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		HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
		MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
		SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UΖ,	VN,	YU,	ZA,
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	NO 200	10041	34	Α		2001	1022		NO	20	01-4	134		2001	0824		
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PRIO	RITY AP	PLN.	INFO	. :				1	JP 19	999-	3690	08	Α	1999	1227		
			٠					1	WO 20	000-	JP91	31	W	2000	1222		
								9	JP 20	000-	3919	)4	Α	2000	1225		
								<u> </u>	JP 20	001-	1937	36	Α	2001	0626		
OTHE	R SOURC	E(S):			MAR	PAT :	135:7	7687	4								

GΙ

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011  $\mu$ M against hepatitis C virus polymerase. A formulation is given.

### IT 347165-90-6P

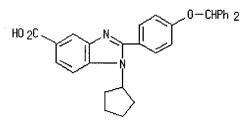
CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heterocyclic compds. as remedies for hepatitis C)

# RN <u>347165-90-6</u> HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 1-cyclopentyl-2-[4-(diphenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

27



REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold									
COST IN U.S. DOLLARS	SINCE FILE	TOTAL							
	ENTRY	SESSION							
FULL ESTIMATED COST	33.22	435.86							
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL							
	ENTRY	SESSION							
CA SUBSCRIBER PRICE -3.47 -12.48									

FILE 'CAOLD' ENTERED AT 00:50:07 ON 12 MAY 2004
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FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY  $\,$ 

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ring bonds :
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normalized bonds :
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isolated ring systems:
    containing 1 : 11 : 51 : 58 :
G1:C,N
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G2: [\*1], [\*2], [\*3], [\*4], [\*5], [\*6], [\*7], [\*8], [\*9], [\*10]

G3:Cy,[\*11],[\*12],[\*13],[\*14]

G4:H,F,CH3,NH2

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS 72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS 87:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS 99:CLASS 99:CLASS

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xact/norm bonds 5-8 6-10 8-9 9-10 9-13 11-12 3-4 3-66 4-5 4-84 5-6 1-2 2-85 **1-**6 2-3 19-20 19-23 11-89 12-13 12-88 13-14 14-15 14-87 15-16 15-90 16-17 17-82 31-35 34-35 37 - 3832 - 3333 - 3425-26 25-29 26-27 27 - 2828-29 31-32 21-22 22-23 51-55 52-53 53-54 53-56 54-55 46-48 48-49 51-52 37-39 39-40 42-43 42-45 46-47 71-72 59-60 60-61 60-63 61-62 67-68 70-71 74-75 75-76 78-79 91 - 9258-59 58-62 92-94 97-98 98-99 92-93 96-97 solated ring systems : containing 1 : 11 : 51 : 58 :

1:C,N

2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6],[\*7],[\*8],[\*9],[\*10]

3:Cy,[\*11],[\*12],[\*13],[\*14]

4:H,F,CH3,NH2

5:C,N -

ch level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS 42:CLASS 43:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:CLASS 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:CLASS 66:CLASS 67:Atom 68:CLASS 70:CLASS 71:CLASS 72:Atom 74:CLASS 75:CLASS 76:CLASS 78:CLASS 79:CLASS 82:CLASS 84:CLASS 85:CLASS 87:CLASS 88:CLASS 89:CLASS 90:CLASS 91:CLASS 92:CLASS 93:CLASS 94:CLASS 96:CLASS 97:CLASS 98:CLASS 99:CLASS

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			and searchable
NEWS 4	JAN	27 .	A new search aid, the Company Name Thesaurus, available in CA/CAplus
NEWS 5	FEB	05	German (DE) application and patent publication number format
NEMO 2	rud	03	changes
NEWS 6	MAR	0.3	MEDLINE and LMEDLINE reloaded
NEWS 7	MAR		MEDLINE file segment of TOXCENTER reloaded
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NEWS 11	MAR	29	New monthly current-awareness alert (SDI) frequency in RAPRA
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NEWS 13	APR	26	<pre>IFIPAT/IFIUDB/IFICDB: New super search and display field</pre>
			available
	APR		LITALERT now available on STN
	APR		NLDB: New search and display fields available
NEWS 16	May		PROUSDDR now available on STN
NEWS 17	May	19	PROUSDDR: One FREE connect hour, per account, in both May
NEWS 18	Marr	12	and June 2004 EXTEND option available in structure searching
	May May		Polymer links for the POLYLINK command completed in REGISTRY
NEWS 19	May	14	Polymer Times for the robibline command completed in Abereria
NEWS EXP	RESS	MA	RCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
			CINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
•		AN	D CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
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=> file reg COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

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STRUCTURE FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4 DICTIONARY FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

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Experimental and calculated property data are now available. For more information enter <a href="http://example.com/HELP\_PROP">HELP\_PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

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STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

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H 92 F 93 C 93 N M2

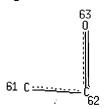
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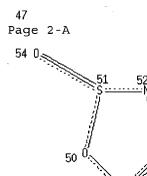
Page 1-D



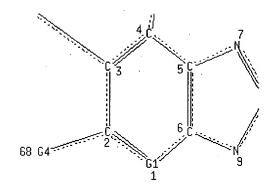
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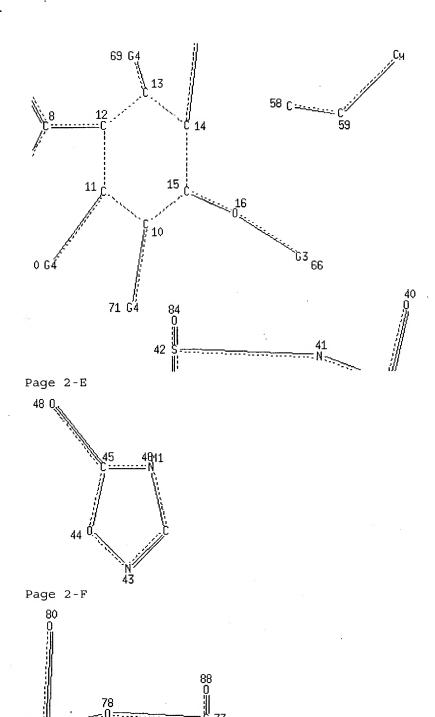
Page 1-E



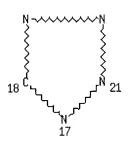
Page 2-B



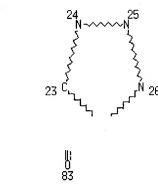
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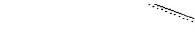


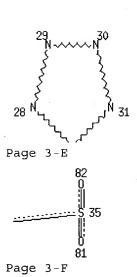
Page 3-B

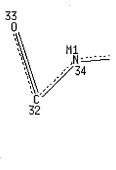


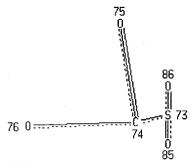
Page 3-D









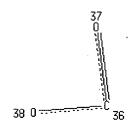


Page 4-B



Page 4-D

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Page 4-E VAR G1=89/90

VAR G2=18/24/29/35/36/42/47/53/73/77

VAR G3=91/57/58/61/64

VAR G4=92/93/94/95

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HCOUNT	IS	M1	AT	46
HCOUNT	IS	M1	AT	52
HCOUNT	IS	М3	TA	94
HCOUNT	IS	M2	ΑT	95
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
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         61 62 63 64 65 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88
         91 92 93 94 95
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC 10 8 43 49
NUMBER OF NODES IS 95
STEREO ATTRIBUTES: NONE
=> s 11
SAMPLE SEARCH INITIATED 15:56:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 302 TO ITERATE
100.0% PROCESSED
                  302 ITERATIONS
                                                           37 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS: 4998 TO 7082
PROJECTED ANSWERS:
                            376 TO
            37 SEA SSS SAM L1
1.2
=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N or END:y
FULL SEARCH INITIATED 15:56:16 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6058 TO ITERATE
100.0% PROCESSED
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                                                          599 ANSWERS
SEARCH TIME: 00.00.02
           599 SEA SSS FUL L1
L3
=> file hcaplus
COST IN U.S. DOLLARS
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FULL ESTIMATED COST
                                                  156.26
                                                           156.47
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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 11 May 2004 (20040511/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4 14 L3

=> s 14 and beaulieu, p?
50 BEAULIEU .

TERM 'P?' EXCEEDED TRUNCATION LIMITS - SEARCH ENDED You have entered a truncated stem which occurs in too many terms. Make the stem longer and try again. For example, if your original term was 'degr?' to search for variations and the abbreviation for 'degradation', you could replace it with the expression '(degrdn OR degrad?)'. If your search term was numeric, e.g., 'C>5', reduce the size of the range.

 $\Rightarrow$  d 15, ibib abs fhitstr, 1-2

L5 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

140:246106



ACCESSION NUMBER:

2003:981461 HCAPLUS

DOCUMENT NUMBER:

Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of

benzimidazole derivatives

AUTHOR(S):

TITLE:

Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves; Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet,

Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin,

Charles; Austel, Volkhard; Kukolj, George

CORPORATE SOURCE: Department of Chemistry, Research and Development,

Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S

2G5, Can.

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2004),

14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

IT 390815-16-4P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

390815-16-4 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS 21 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2002:51438 HCAPLUS

DOCUMENT NUMBER:

136:118447

TITLE:

Preparation of benzimidazolecarboxylates and related

compounds as viral polymerase inhibitors

INVENTOR(S):

Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard,

James; Kukolj, George; Austel, Volkhard Boehringer Ingelheim (Canada) Ltd., Can.

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 322 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	I	APPLICATION NO.	DATE
WO 2002004425	A2 20020	0117	NO 2001-CA989	20010704
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OTHER SOURCE(S):

MARPAT 136:118447

GΙ

Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH2, NMeR3, NHR3, OR3, 5-6 AΒ membered (substituted) heterocyclyl; A = N, COR7, CR5; R5 = H, halo, alkyl; R7 = H, alkyl; X and A are not both N; R6 = H, halo, alkyl, OR7; R7 = H , alkyl; R1 = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF3; R2 = (substituted) alkyl, cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. qiven), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5  $\mu$ M.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

RN 347166-09-0 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)

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STRUCTURE FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4 DICTIONARY FILE UPDATES: 11 MAY 2004 HIGHEST RN 681211-23-4

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter <a href="HELP PROP">HELP PROP</a> at an arrow prompt in the file or refer to the file summary sheet on the web at: <a href="http://www.cas.org/ONLINE/DBSS/registryss.html">http://www.cas.org/ONLINE/DBSS/registryss.html</a>

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The previous command name entered was not recognized by the system.
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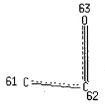
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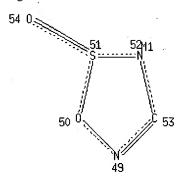


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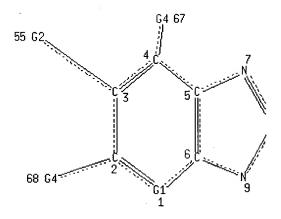


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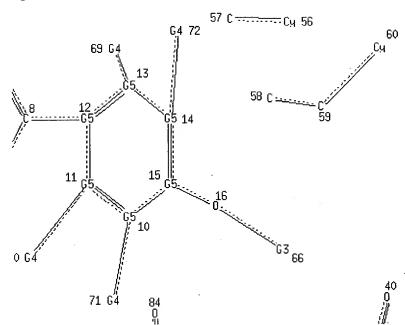
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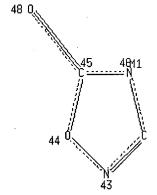


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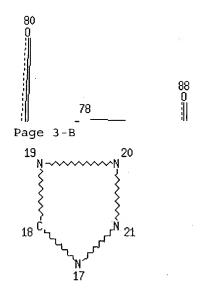


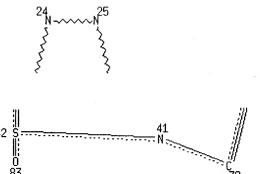
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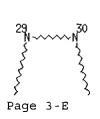
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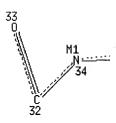
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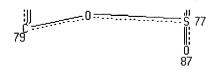


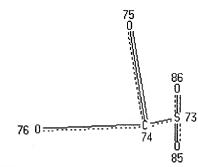
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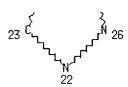


Page 3-F





Page 4-B



Page 4-D





Page 4-E
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FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*
PROJECTED ITERATIONS: 38265 TO 43695
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L7 19 SEA SSS SAM L6

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L8

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

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FILE COVERS 1907 - 12 May 2004 VOL 140 ISS 20 FILE LAST UPDATED: 11 May 2004 (20040511/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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14 L8

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8 L8/THU

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ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN L9

Full Text ACCESSION NUMBER:

2003:981461 HCAPLUS

DOCUMENT NUMBER: 140:246106

Non-nucleoside inhibitors of the hepatitis C virus NS5B polymerase: discovery and preliminary SAR of

benzimidazole derivatives

AUTHOR(S): Beaulieu, Pierre L.; Bos, Michael; Bousquet, Yves;

TITLE:

Fazal, Gulrez; Gauthier, Jean; Gillard, James; Goulet,

Sylvie; LaPlante, Steven; Poupart, Marc-Andre; Lefebvre, Sylvain; McKercher, Ginette; Pellerin,

Charles; Austel, Volkhard; Kukolj, George

CORPORATE SOURCE: Department of Chemistry, Research and Development,

Boehringer Ingelheim (Canada) Ltd., Laval, QC, H7S

2G5, Can.

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004),

14(1), 119-124

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier Science B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Benzimidazole 5-carboxamide derivs. from a combinatorial screening library were discovered as specific inhibitors of the NS5B polymerase of the hepatitis C virus (HCV). Initial hit-to-lead activities taking advantage of high-throughput parallel synthetic techniques, identified a 1,2-disubstituted benzimidazole 5-carboxylic acid scaffold as the min. core for biol. activity. Potent analogs in this series inhibit the polymerase at low micromolar concns. and provide an attractive 'drug-like' lead structure for further optimization and the development of potential HCV therapeutics.

IT 390815-16-4P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery and preliminary SAR of benzimidazole derivs. as inhibitors of hepatitis C virus NS5B polymerase)

RN 390815-16-4 HCAPLUS

> 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-[2-[[3-(dimethylamino)propyl]amino]-2-oxoethoxy]phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Sintar

ACCESSION NUMBER: DOCUMENT NUMBER:

2003:970508 HCAPLUS

140:174511

TITLE:

Mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of the hepatitis C virus RNA-dependent RNA polymerase Tomei, Licia; Altamura, Sergio; Bartholomew, Linda; Biroccio, Antonino; Ceccacci, Alessandra; Pacini,

AUTHOR(S):

Laura; Narjes, Frank; Gennari, Nadia; Bisbocci, Monica; Incitti, Ilario; Orsatti, Laura; Harper, Steven; Stansfield, Ian; Rowley, Michael; De Francesco, Raffaele; Migliaccio, Giovanni

CORPORATE SOURCE:

Istituto di Ricerche di Biologia Molecolare "P.

Angeletti", Pomezia-Rome, 00040, Italy

SOURCE:

Journal of Virology (2003), 77(24), 13225-13231

CODEN: JOVIAM; ISSN: 0022-538X

PUBLISHER: DOCUMENT TYPE: American Society for Microbiology

Journal LANGUAGE: English

The RNA-dependent RNA polymerase of hepatitis C virus (HCV) is the catalytic subunit of the viral RNA amplification machinery and is an appealing target for the development of new therapeutic agents against HCV infection. Nonnucleoside inhibitors based on a benzimidazole scaffold have been recently reported. Compds. of this class are efficient inhibitors of HCV RNA replication in cell culture, thus providing attractive candidates for further development. Here we report the detailed anal. of the mechanism of action of selected benzimidazole inhibitors. Kinetic data and binding expts. indicated that these compds. act as allosteric inhibitors that block the activity of the polymerase prior to the elongation step. Escape mutations that confer resistance to these compds. map to proline 495, a residue located on the surface of the polymerase thumb domain and away from the active site. Substitution of this residue is sufficient to make the HCV enzyme and replicons resistant to the inhibitors. Interestingly, proline 495 lies in a recently identified noncatalytic GTP-binding site, thus validating it as a potential allosteric site that can be targeted by small-mol. inhibitors of HCV polymerase.

IT 658693-60-8

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (mechanism of action and antiviral activity of benzimidazole-based allosteric inhibitors of hepatitis C virus RNA-dependent RNA polymerase)

658693-60-8 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 2-[4-[[4'-chloro-4-[(4-hydroxy-1-CN piperidinyl)carbonyl][1,1'-biphenyl]-2-yl]methoxy]-2-fluorophenyl]-1cyclohexyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

1.9 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Citina ACCESSION NUMBER:

2003:319709 HCAPLUS

DOCUMENT NUMBER:

138:338144

TITLE:

Preparation of 2-phenyl benzimidazoles and

imidazo-[4,5]pyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in the

treatment of cancer

INVENTOR(S):

Arienti, Kristen L.; Axe, Frank U.; Breitenbucher, J.

Guy; Huang, Liming; Lee, Alice; McClure, Kelly J.

PATENT ASSIGNEE(S):

Ortho-McNeil Pharmaceutical, Inc., USA

SOURCE:

PCT Int. Appl., 144 pp.

DOCUMENT TYPE:

CODEN: PIXXD2 Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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OTHER S		MΔP	ייעם	138.	ว ว ภ า .	1 4												

OTHER SOURCE(S):

MARPAT 138:338144

I

GT

AΒ 2-Aryl-substituted benzimidazoles and imidazo[4,5]pyridines (shown as I; e.g. 2-[4-(4-chlorophenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide (II)) are disclosed as inhibitors of Cds1 and useful as adjuvants to chemotherapy or radiation therapy in the treatment of cancer. For I: W is COOH, -C(0)NHR1, or -SO2NHR1 (R1 is H or C1-4alkyl); Q is N or CH; Ra and Rb are H or halogen; Y, Y1 and Y2 = N and C-Rc with the proviso that 0, 1or 2 of Y, Y1 and Y2 are N and at least 2 of Rc must be H; Rc = -H, -OH, -C1-6alkyl, -SCF3, halo, -CF3 and -OCF3; Z = O, S, SO, SO2, SO2NR2, NR2SO2, NH, CONR2, piperazinediyl or a covalent bond; R2 is H or C1-4alkyl; Ar1 is an arom. group as defined in the claims. IC50 values are reported for inhibition of human Cds1 checkpoint kinase by 103 examples of I, e.g. 3 nM for 2-[4-(4-chloro-3trifluoromethylphenoxy)phenyl]-1H-benzimidazole-5-carboxylic acid amide.

Addnl. studies were (i) detn. of the effect of II on tumor cell line clonogenic survival, (ii) effect of II on tumor growth in murine xenograft models, (iii) detn. of the effect of 14 examples of I on radiation-induced apoptosis in isolated primary cells, and (iv) detn. of the effect of II on radiation-induced apoptosis in splenocytes in vivo. Although the methods of prepn. are not claimed, ~100 example prepns. are included.

IT 516480-80-1P, 2-[4-(4-Chlorophenoxy)phenyl]-1H-benzimidazole-5carboxylic acid

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; prepn. of benzimidazoles and imidazopyridines as Cds1/Chk2-inhibitors and adjuvants to chemotherapy or radiation therapy in treatment of cancer)

RN 516480-80-1 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(4-chlorophenoxy)phenyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

## L9 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:261620 HCAPLUS

138:287673

DOCUMENT NUMBER: TITLE:

Preparation of phenylbenzimidazole compounds useful

for treating hepatitis C virus

INVENTOR(S):

Priestley, Eldon Scott; Decicco, Carl P.; Hudyma,

Thomas W.; Zheng, Xiaofan

PATENT ASSIGNEE(S):

Bristol-Myers Squibb Company, USA

SOURCE:

PCT Int. Appl., 74 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	ז ת ת	APPLICATION NO. DATE								
PAIENI NO.	KIND DATE	API	PLICATION NO.	DATE							
WO 2003026587	A2 20030	403 <u>WO</u>	WO 2002-US30989 20020926								
WO 2003026587	A3 20031	106									
W: AE, AG,	AL, AM, AT,	AU, AZ, BA, B	BB, BG, BR, BY,	BZ, CA, CH, CN,							
CO, CR,	CU, CZ, DE,	DK, DM, DZ, H	EC, EE, ES, FI,	GB, GD, GE, GH,							
GM, HR,	HU, ID, IL,	IN, IS, JP, H	KE, KG, KP, KR,	KZ, LC, LK, LR,							
LS, LT,	LU, LV, MA,	MD, MG, MK, N	MN, MW, MX, MZ,	NO, NZ, OM, PH,							
PL, PT,	RO, RU, SD,	SE, SG, SI, S	SK, SL, TJ, TM,	TN, TR, TT, TZ,							
UA, UG,	UZ, VN, YU,	ZA, ZM, ZW, A	AM, AZ, BY, KG,	KZ, MD, RU, TJ, TM							
RW: GH, GM,	KE, LS, MW,	MZ, SD, SL, S	SZ, TZ, UG, ZM,	ZW, AT, BE, BG,							
CH, CY,	CZ, DE, DK,	EE, ES, FI, H	FR, GB, GR, IE,	IT, LU, MC, NL,							
PT, SE,	SK, TR, BF,	BJ, CF, CG, C	CI, CM, GA, GN,	GQ, GW, ML, MR,							
NE, SN,	TD, TG	• -	•								
US 2003134853	A1 20030	717 US	US 2002-259041 20020926								

US 2004067976 PRIORITY APPLN. INFO.:

20040408 Α1

20030827 US 2003-648873

US 2001-324874P P 20010926

B1 20020926

OTHER SOURCE(S):

US 2002-259041 MARPAT 138:287673

$$R^1$$
 $R^3$ 
 Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, AB etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14  $\mu M$  against HCV NS5B RdRp (RNA-dependent RNA polymerase).

IT 503857-56-5P

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of phenylbenzimidazole compds. for treating hepatitis C viral infection)

503857-56-5 HCAPLUS RN

Glycine, N-[4-(5-acetyl-2-thienyl)-3-[[4-[1-cyclohexyl-5-(1H-tetrazol-5-CNyl)-1H-benzimidazol-2-yl]phenoxy]methyl]benzoyl]-, 1,1-dimethylethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 503857-55-4 CMF C40 H41 N7 O5 S

CM 2

CRN  $\frac{76-05-1}{C2 H F3}$  O2

F-C-C0 2F

L9 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Clang Text References

ACCESSION NUMBER:

2003:203407 HCAPLUS

DOCUMENT NUMBER:

138:238181

TITLE:

Preparation of substituted 1-cyclohexyl-2-

phenylbenzimidazole-5-carboxylic acids as remedies for

hepatitis C

INVENTOR(S):

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S):

Japan Tobacco Inc., Japan

SOURCE:

U.S. Pat. Appl. Publ., 406 pp., Cont.-in-part of Appl.

No. PCT/JP00/09181.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	Ξ	APPLICATION NO	D. DATE				
US 2003050320	A1 2003	30313	US 2001-939374	20010824				
WO 2001047883	A1 2001	L0705	WO 2000-JP918:	20001222				
W: AE, AG	, AL, AM, AT,	AU, AZ,	BA, BB, BG, BR,	BY, BZ, CA, CH, CN,				
· CR, CU	, CZ, DE, DK,	DM, DZ,	EE, ES, FI, GB,	GD, GE, GH, GM, HR,				
HU, · ID	, IL, IN, IS,	KE, KG,	KR, KZ, LC, LK,	LR, LS, LT, LU, LV,				
MA, MD	, MG, MK, MN,	MW, MX,	MZ, NO, NZ, PL,	PT, RO, RU, SD, SE,				
SG, SI	, SK, SL, TJ,	TM, TR,	TT, TZ, UA, UG,	US, UZ, VN, YU, ZA,				
ZW, AM	, AZ, BY, KG,	KZ, MD,	RU, TJ, TM					
RW: GH, GM	, KE, LS, MW,	MZ, SD,	SL, SZ, TZ, UG,	ZW, AT, BE, CH, CY,				
DE, DK	, ES, FI, FR,	GB, GR,	IE, IT, LU, MC,	NL, PT, SE, TR, BF,				
BJ, CF	, CG, CI, CM,	GA, GN,	GW, ML, MR, NE,	SN, TD, TG				
JP 2001247550	A2 2001	10911	JP 2000-391904	20001225				
PRIORITY APPLN. INF	O.:	ن	JP 1999-369008	A 19991227				
		$\overline{V}$	WO 2000-JP9181	A2 20001222				
			JP 2000-391904	A 20001225				
			JP 2001-193786 A 20010626					
OTHER SOURCE(S):	MARPAT	31						

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5,

G6, G8, G9 = C, N; G7 = O, S, CR7, etc.; R1-R4 = H, NO2, etc.; ring Cy =(un) substituted cycloalkyl ring, etc.; ring A = Ph, cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, CN, etc.; R7 = H, alkyl] are prepd. and formulated. Compds. I showed HCV polymerase inhibitory activity (data given). E.g., a multi-step synthesis of II.HCl, starting from 2-bromo-5-nitrotoluene and Me 2-(2-fluoro-4-hydroxyphenyl)-1cyclohexylbenzimidazole-5-carboxylate, was given.

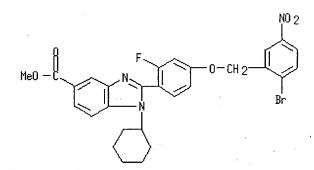
IT 480461-26-5P

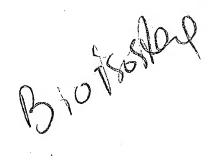
CN

RL: PAC (Pharmacological activity); RCT (Reactant); THU (Therapeutic use); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of substituted 1-cyclohexyl-2-phenylbenzimidazole-5-carboxylic acids as remedies for hepatitis C)

480461-26-5 HCAPLUS . RN

> 1H-Benzimidazole-5-carboxylic acid, 2-[4-[(2-bromo-5-nitrophenyl)methoxy]-2-fluorophenyl]-1-cyclohexyl-, methyl ester (9CI) (CA INDEX NAME)





ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

e Citine) Full References

ACCESSION NUMBER: 2003:5773 HCAPLUS

DOCUMENT NUMBER: 138:66657

TITLE: Fused cyclic compounds and medicinal use thereof

INVENTOR(S): Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida,

Atsuhito

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan

SOURCE: PCT Int. Appl., 603 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

מעם	יייאלים י	NIO		עדי	ATD.	DATE APPLICATION NO.							^	ከእጥሮ				
PAI	LENI .	NO.		VTI	ND .	DATE AFFEICATION NO. DATE												
WO 2003000254 A1				1	2003	0103		WO 2002-JP6405					20020626					
	W:	ΑE,	AG,	ΑL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	
		LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	PL,	PT,	
		RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	
		US,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	AZ,	BY,	KG,	ΚZ,	MD,	RU,	TJ,	TM	
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,	
		CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
JP	P 2003212846 A2				2	20030730			<u>J</u>	JP 2002-185241				20020625				
BR	BR 2002005684			Α		2003	0617		BR 2002-5684					20020626				

EP 1400241 Α1 20040324 EP 2002-743728 20020626 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR US 2003-344997 US 2004082635 A1 20040429 20030218 NO 2003000832 20030422 20030221 NO 2003-832 PRIORITY APPLN. INFO.: JP 2001-193786 A 20010626 JP 2001-351537 A 20011116 WO 2002-JP6405 W 20020626

OTHER SOURCE(S):

MARPAT 138:66657

GI

AB Fused cyclic compds. represented by the following general formula [I] or pharmaceutically acceptable salts thereof and remedies for hepatitis C contg. these compds.: I wherein each symbol is as defined in the description. Because of having an effect against hepatitis C virus (HVC) based on an HCV polymerase inhibitory effect, these compds. are useful as remedies or preventives for hepatitis C.

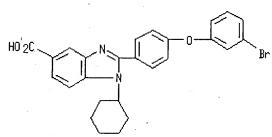
IT 347165-35-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fused cyclic compds. as hepatitis C virus polymerase inhibitors and antiviral agents)

RN 347165-35-9 HCAPLUS

CN 1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1-cyclohexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN

Text References
ACCESSION NUMBER:

2002:51438 HCAPLUS

DOCUMENT NUMBER:

136:118447

TITLE:

Preparation of benzimidazolecarboxylates and related

compounds as viral polymerase inhibitors

INVENTOR(S): Beaulieu, Pierre Louis; Fazal, Gulrez; Gillard, James;

Kukolj, George; Austel, Volkhard

PATENT ASSIGNEE(S):

Boehringer Ingelheim (Canada) Ltd., Can.

SOURCE:

PCT Int. Appl., 322 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

PATENT NO. DATE APPLICATION NO. KIND ----------**-----**\_\_\_\_\_ WO 2001-CA989 WO 2002004425 A2 20020117 20010704 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 2001-898297 20010703 US 2002065418 20020530 Al 20020910 US 6448281 EP 2001-951274 EP 1301487 20030416 20010704 Α2 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR JP 2002-509292 20010704 JP 2004502761 T2 20040129 US 6479508 20021112 US 2001-995099 20011127 B1 WO 2002-CA323 A2 20020912 20020306 WO 2002070739 WO 2002070739 Α3 20030530 AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG EP 2002-712681 20031217 EP 1370682 A2 20020306 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR A1 20031218 20020910 US 2003232816 US 2002-238282 PRIORITY APPLN. INFO.: US 2000-216084P P 20000706 US 2001-274374P Ρ 20010308 US 2001-281343P P 20010405 US 2001-898297 A3 20010703 WO 2001-CA989 20010704 W US 2001-995099 A3 20011127 WO 2002-CA323 W 20020306

OTHER SOURCE(S):

MARPAT 136:118447

R1 A (CH 2) nCY

Title compds. [I; X = CH, N; Y = O, S; Z = OH, NH2, NMeR3, NHR3, OR3, S-6AΒ membered (substituted) heterocyclyl; A = N, COR7, CR5; R5 = H, halo, alkyl; R7 = H, alkyl; X and A are not both N; R6 = H, halo, alkyl, OR7; R7 = H , alkyl; R1 = (substituted) hetero(bi)cyclyl, Ph, phenylalkyl, alkenyl, phenylalkenyl, cycloalkyl, alkyl, CF3; R2 = (substituted) alkyl, cycloalkyl, cycloalkylalkyl, bicycloalkyl, adamantyl, Ph, pyridyl; R3 = H, alkyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, alkenyl, cycloalkylalkenyl, arylalkenyl, dialkylamino, heterocyclyl, etc.; n = 0, 1], were prepd. Thus, Me 3-amino-4-cyclohexylaminobenzoate (prepn. given), 2-pyridinecarboxaldehyde, and Oxone were stirred in DMF to give 80% Et 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylate, which was sapond. with aq. NaOH in MeOH to give 91% 1-cyclohexyl-2-pyridin-2-yl-1H-benzimidazole-5-carboxylic acid. The latter inhibited hepatitis C virus RNA dependent polymerase (NS5B) with IC50 = 1-5 uM.

IT 347166-09-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of benzimidazolecarboxylates and related compds. as viral polymerase inhibitors)

347166-09-0 HCAPLUS RN

1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[4-CN (phenylmethoxy)phenyl] - (9CI) (CA INDEX NAME)

ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2004 ACS on STN L9

ACCESSION NUMBER: 2001:489367 HCAPLUS

DOCUMENT NUMBER: 135:76874

Preparation of heterocyclic compounds as remedies for TITLE:

hepatitis C

Hashimoto, Hiromasa; Mizutani, Kenji; Yoshida, INVENTOR(S):

Japan Tobacco Inc., Japan

Atsuhito

SOURCE: PCT Int. Appl., 438 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

Japanese LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

PATENT NO.				KI	ND I	DATE			A.	PPLI	CATI	ON NC	o. :	DATE				
								-										
WO 2001047883				A	1	2001	0705		WO 2000-JP9181					20001222				
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							DK,											
			HU,	ID,	IL,	IN,	IS,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,
			MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
			SG.	ST.	SK.	SL.	TJ.	TM.	TR.	TT.	TZ.	UA.	UG,	US,	UZ,	VN,	YU,	ZA,

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             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                           EP 2000-987728
                            20011212
                                                             20001222
                       Α1
    EP 1162196
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                                             20001222
                            20020102
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     BR 2000008525
                       Α
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                       T1
                                            NZ 2000-514403
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    NZ 514403
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                            20021025
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     AU 763356
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                                            RU 2001-126283
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                       C2
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                            20011022
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     NO 2001004134
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                           20030313
                                            US 2001-939374
     US 2003050320
                       Α1
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                                            ZA 2001-7870
                                                             20010928
     ZA 2001007870
                                         JP 1999-369008
                                                             19991227
PRIORITY APPLN. INFO.:
                                         WO 2000-JP9181
                                                          W 20001222
                                         JP 2000-391904
                                                             20001225
                                                          Α
                                                             20010626
                                         JP 2001-193786
                                                          Α
```

OTHER SOURCE(S):

MARPAT 135:76874

GΙ

The title compds. I [the dotted line in rings B1 and B2 indicates a single or double bond; G1 = N, CR1; G2 = N, CR2, G3 = N, CR3; G4 = N, CR4; G5, G6, G8, G9 = C, N; G7 = O, etc.; R1 - R4 = H, nitro, etc.; ring Cy = (un)substituted cycloalkyl ring, etc.; ring A = C3-C8 cycloalkyl, etc. R5, R6 = H, halo, etc.; X = H, cyano, etc.] are prepd. The benzimidazole deriv. II in vitro showed IC50 of 0.011 μM against hepatitis C virus polymerase. A formulation is given.

IT 347165-35-9P

RN

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heterocyclic compds. as remedies for hepatitis C)

347165-35-9 HCAPLUS

1H-Benzimidazole-5-carboxylic acid, 2-[4-(3-bromophenoxy)phenyl]-1cyclohexyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION 42.77 386.37 FULL ESTIMATED COST TOTAL DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY SESSION -5.54 -6.93 CA SUBSCRIBER PRICE

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27

FILE COVERS 1907-1966 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter  $\underline{\text{HELP FIRST}}$  for more information.

## => d his

(FILE 'HOME' ENTERED AT 15:54:32 ON 12 MAY 2004)

FILE 'REGISTRY' ENTERED AT 15:54:39 ON 12 MAY 2004

L1 STRUCTURE UPLOADED

L2 37 S L1

L3 599 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 15:56:23 ON 12 MAY 2004

L4 14 S L3

L5 2 S L4 AND BEAULIEU, P?/AU

FILE 'REGISTRY' ENTERED AT 15:58:17 ON 12 MAY 2004

L6 STRUCTURE UPLOADED

L7 19 S L6

L8599 S L6 FULL

FILE 'HCAPLUS' ENTERED AT 16:20:18 ON 12 MAY 2004 L9 8 S L8/THU

FILE 'CAOLD' ENTERED AT 16:21:23 ON 12 MAY 2004

L10 0 L3